Computational Science II
-
FS15 Project / Daniel Studer

Improving the computation time

Algorithm of force.f90

First Algorithm

Formula:

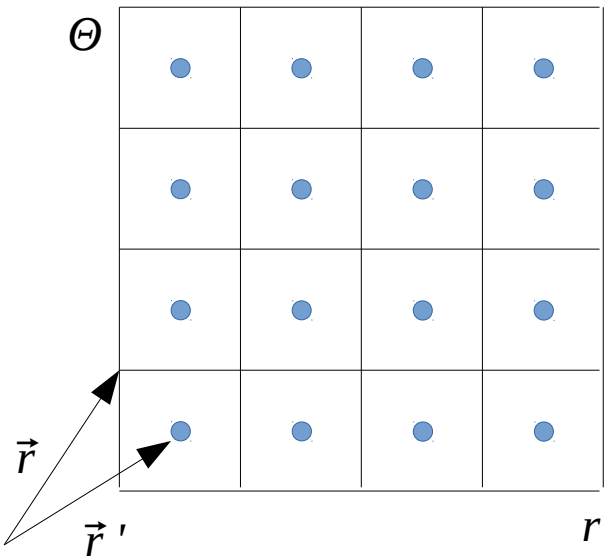
$$\vec{F}(\vec{r}) = -\iint \frac{G\,\rho(\vec{r})\,r'\,dr'\,d\Theta'}{\left|r^2 + r'^2 - 2rr'\cos(\Theta-\Theta')\right|^{3/2}} \begin{pmatrix} r - r'\cos(\Theta-\Theta') \\ r'\sin(\Theta-\Theta') \end{pmatrix}$$

Loading:
- density_project.data → ρ [256,128]
- r_project.data → r' [128]
- theta_project.data → Θ' [256]

Calculating:
- dr, dΘ
- r [129]
- Θ [257]

Loop: for 129*257 points 128*256 times

Required Time ~ 125.73 s



Algorithm of force.f90

Second Algorithm

Formula: $$\vec{F}(\vec{r}) = -\iint \frac{G\rho(\vec{r})\, r'\, dr'\, d\Theta'}{\left|r^2 + r'^2 - 2rr'\cos(\Theta - \Theta')\right|^{3/2}} \begin{pmatrix} r - r'\cos(\Theta - \Theta') \\ r'\sin(\Theta - \Theta') \end{pmatrix}$$

Loading:
- density_project.data → ρ [256,128]
- r_project.data → r' [128]
- theta_project.data → Θ' [256]

Calculating:
- dr, dΘ
- r [129]
- Θ [257]
- cos(Θ-Θ') → cosdΘ [257,256]
- sin(Θ-Θ') → sindΘ [257,256]

Loop: for 129*257 points 128*256 times

Required Time ~ 40.77 s

Algorithm of force.f90

Third Algorithm

Formula:

$$\vec{F}(\vec{r}) = -\iint \frac{G\,\rho(\vec{r})\,r'\,dr'\,d\Theta'}{\left|r^2 + r'^2 - 2rr'\cos(\Theta-\Theta')\right|^{3/2}} \begin{pmatrix} r - r'\cos(\Theta-\Theta') \\ r'\sin(\Theta-\Theta') \end{pmatrix}$$

Loading:
- density_project.data → ρ [256,128]
- r_project.data → r' [128]
- theta_project.data → Θ' [256]

Calculating:
- dr, dΘ
- r [129]
- Θ [257]
- cos(Θ-Θ') → cosdΘ [257,256]
- sin(Θ-Θ') → sindΘ [257,256]

Substitution:
- R = r/r' → R [129,128]
- dR= -r/r'² dr' → dR[129,128]

Algorithm of force.f90

Third Algorithm

Formula: $$\vec{F}(\vec{r}) = -\iint \frac{G\,\rho(\vec{r})\,dR\,d\Theta'}{R\left|R^2+1-2R\cos(\Theta-\Theta')\right|^{3/2}} \begin{pmatrix} R-\cos(\Theta-\Theta') \\ \sin(\Theta-\Theta') \end{pmatrix}$$

Loading:
- density_project.data → ρ [256,128]
- r_project.data → r' [128]
- theta_project.data → Θ' [256]

Calculating:
- dr, dΘ
- r [129]
- Θ [257]
- cos(Θ-Θ') → cosdΘ [257,256]
- sin(Θ-Θ') → sindΘ [257,256]

Substitution:
- R = r/r' → R [129,128]
- dR= -r/r'² dr' → dR[129,128]

Loop: for 129*257 points 128*256 times

Source Code force.f90

```
program forcefield
implicit none

! initialize variables and grids        _____________________________________

integer::dim_r,dim_theta
integer::dim_r1,dim_theta1
integer::i,j,k,l
real::t_start,t_end,t
real::var0,var1,var2,var3,var4,var5,var6
real::G
real::dr,dtheta
real::dforce_r,dforce_theta
real,dimension(256+1,256)::cos_dtheta
real,dimension(256+1,256)::sin_dtheta
real,dimension(128+1,128)::r_sub
real,dimension(128+1,128)::dr_sub
real,dimension(128)::r
real,dimension(256)::theta
real,dimension(128+1)::r1
real,dimension(256+1)::theta1
real,dimension(128,256)::density
real,dimension(128+1,256+1,2)::force
G=1
dim_theta=256
dim_r=128
dim_theta1=dim_theta+1
dim_r1=dim_r+1

!_____________________________________________________________________
```

Source Code force.f90

```
! load data from Computational_Science_II/Data/    _____

open(unit=1,file="Data/r_project.data")
do i=1,dim_r
        read(1,'(e20.10)') r(i)
end do
close(1)
open(unit=2,file="Data/theta_project.data")
do i=1,dim_theta
        read(2,'(e20.10)') theta(i)
end do
close(2)
open(unit=3,file="Data/density_project.data")
do i=1,dim_r
        do k=1,dim_theta
                read(3,'(e20.10)') density(i,k)
        end do
end do
Close(3)

!_____________________________________________________________________
```

Source Code force.f90

```
! build theta1, cos_dtheta and sin_dtheta grid      _____

dtheta=theta(2)-theta(1)
do j=1,dim_theta
        theta1(j)=theta(j)-dtheta*0.5
end do
theta1(dim_theta1)=theta(dim_theta)+dtheta*0.5
do j=1,dim_theta1
        do l=1,dim_theta
                var0=theta1(j)-theta(l)
                cos_dtheta(j,l)=cos(var0)
                sin_dtheta(j,l)=sin(var0)
        end do
end do

!_____________________________________________________________________
```

Source Code force.f90

```
! build r1, r_sub and dr_sub grid  _____________________________________

dr=r(2)-r(1)
do i=1,dim_r
        r1(i)=r(i)-dr*0.5
end do
r1(dim_r1)=r(dim_r)+dr*0.5
do i=1,dim_r1
        do k=1,dim_r
                var1=r(k)
                r_sub(i,k)=r1(i)/var1
                dr_sub(i,k)=-r_sub(i,k)/var1*dr
        end do
end do

!_____________________________________________________________________
```

Source Code force.f90

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta
                        var2=cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5=var5*sqrt(var5)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6=var6/var5
                                dforce_r=dforce_r+(var4-var2)*var6
                                dforce_theta=dforce_theta+var3*var6
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________

call CPU_Time(t_end)
t=t_end-t_start
write(*,*) "required time:"
write(*,*) t
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5=var5*sqrt(var5)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6=var6/var5
                                dforce_r=dforce_r+(var4-var2)*var6
                                dforce_theta=dforce_theta+var3*var6
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________

call CPU_Time(t_end)
t=t_end-t_start
write(*,*) "required time:"
write(*,*) t
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var2s=-cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5=var5*sqrt(var5)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6=var6/var5
                                dforce_r=dforce_r+(var4-var2)*var6
                                dforce_theta=dforce_theta+var3*var6
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________

call CPU_Time(t_end)
t=t_end-t_start
write(*,*) "required time:"
write(*,*) t
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var2s=-cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        var3s=-sin_dtheta(j,dim_theta-l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5=var5*sqrt(var5)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6=var6/var5
                                dforce_r=dforce_r+(var4-var2)*var6
                                dforce_theta=dforce_theta+var3*var6
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________

call CPU_Time(t_end)
t=t_end-t_start
write(*,*) "required time:"
write(*,*) t
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var2s=-cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        var3s=-sin_dtheta(j,dim_theta-l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5s=1+var4*var4-2*var4*var2s
                                var5=var5*sqrt(var5)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6=var6/var5
                                dforce_r=dforce_r+(var4-var2)*var6
                                dforce_theta=dforce_theta+var3*var6
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var2s=-cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        var3s=-sin_dtheta(j,dim_theta-l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5s=1+var4*var4-2*var4*var2s
                                var5=var5*sqrt(var5)*var4
                                var5s=var5s*sqrt(var5s)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6=var6/var5
                                dforce_r=dforce_r+(var4-var2)*var6
                                dforce_theta=dforce_theta+var3*var6
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var2s=-cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        var3s=-sin_dtheta(j,dim_theta-l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5s=1+var4*var4-2*var4*var2s
                                var5=var5*sqrt(var5)*var4
                                var5s=var5s*sqrt(var5s)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6s=density(k,l+dim_theta/2)*dr_sub(i,k)
                                var6=var6/var5
                                dforce_r=dforce_r+(var4-var2)*var6
                                dforce_theta=dforce_theta+var3*var6
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var2s=-cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        var3s=-sin_dtheta(j,dim_theta-l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5s=1+var4*var4-2*var4*var2s
                                var5=var5*sqrt(var5)*var4
                                var5s=var5s*sqrt(var5s)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6s=density(k,l+dim_theta/2)*dr_sub(i,k)
                                var6=var6/var5
                                var6s=var6s/var5s
                                dforce_r=dforce_r+(var4-var2)*var6
                                dforce_theta=dforce_theta+var3*var6
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var2s=-cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        var3s=-sin_dtheta(j,dim_theta-l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5s=1+var4*var4-2*var4*var2s
                                var5=var5*sqrt(var5)*var4
                                var5s=var5s*sqrt(var5s)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6s=density(k,l+dim_theta/2)*dr_sub(i,k)
                                var6=var6/var5
                                var6s=var6s/var5s
                                dforce_r=dforce_r+(var4-var2)*var6+(var4-var2s)*var6s
                                dforce_theta=dforce_theta+var3*var6
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var2s=-cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        var3s=-sin_dtheta(j,dim_theta-l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5s=1+var4*var4-2*var4*var2s
                                var5=var5*sqrt(var5)*var4
                                var5s=var5s*sqrt(var5s)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6s=density(k,l+dim_theta/2)*dr_sub(i,k)
                                var6=var6/var5
                                var6s=var6s/var5s
                                dforce_r=dforce_r+(var4-var2)*var6+(var4-var2s)*var6s
                                dforce_theta=dforce_theta+var3*var6+var3s*var6s
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________
```

Source Code force.f90~

```
call CPU_Time(t_start)

! calculate force _____________________________________________________
do j=1,dim_theta1
        do i=1,dim_r1
                dforce_r=0.0
                dforce_theta=0.0
                do l=1,dim_theta/2
                        var2=cos_dtheta(j,l)
                        var2s=-cos_dtheta(j,l)
                        var3=sin_dtheta(j,l)
                        var3s=-sin_dtheta(j,dim_theta-l)
                        do k=1,dim_r
                                var4=r_sub(i,k)
                                var5=1+var4*var4-2*var4*var2
                                var5s=1+var4*var4-2*var4*var2s
                                var5=var5*sqrt(var5)*var4
                                var5s=var5s*sqrt(var5s)*var4
                                var6=density(k,l)*dr_sub(i,k)
                                var6s=density(k,l+dim_theta/2)*dr_sub(i,k)
                                var6=var6/var5
                                var6s=var6s/var5s
                                dforce_r=dforce_r+(var4-var2)*var6+(var4-var2s)*var6s
                                dforce_theta=dforce_theta+var3*var6+var3s*var6s
                        end do
                end do
                force(i,j,1)=dforce_r*dtheta*G
                force(i,j,2)=dforce_theta*dtheta*G
        end do
end do
!_____________________________________________________________________
```

Source Code force.f90/~

```
call CPU_Time(t_end)
t=t_end-t_start
write(*,*) "required time:"
write(*,*) t

! save force_project.data  ____________________________________________
open(unit=4,file="Results/force_project.data")
do i=1,dim_r
        do j=1,dim_theta
                write(4,'(2e20.10)') force(i,j,1) , force(i,j,2)
        end do
end do
close(4)
!_____________________________________________________________________

end program
```

Source Code force.f90

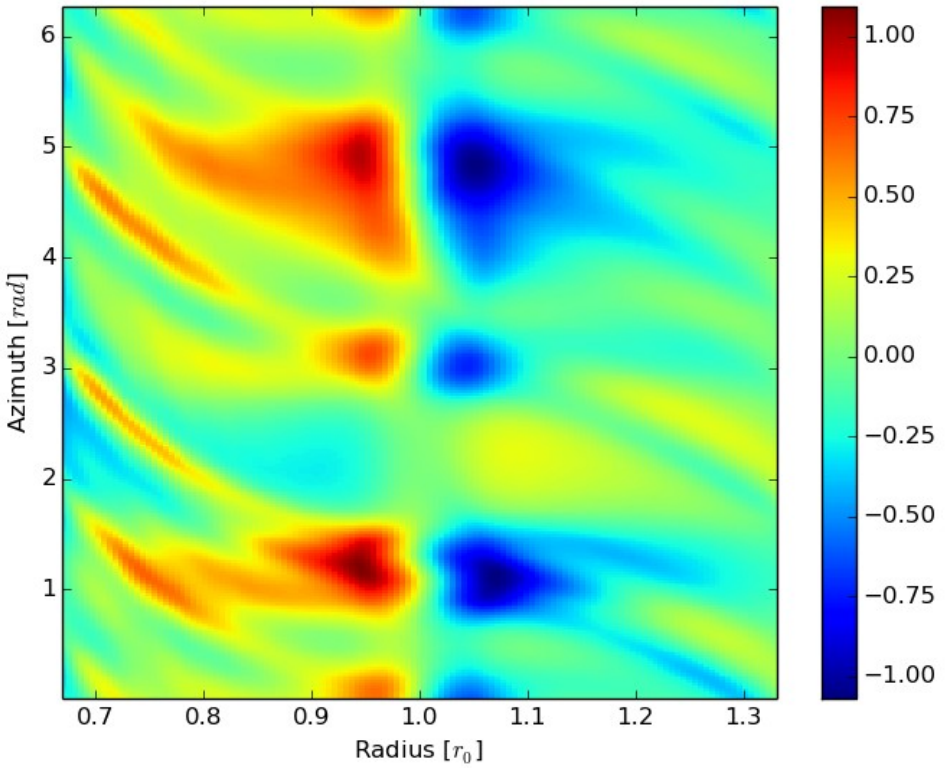
Required Time ~ 36.79 s

Source Code force.f90~

Required Time ~ 30.75 s

Results

r_force.project.data



theta_force.project.data