

grav_project

Computational Science II

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Main assignment

- test of a new algorithm
- gravitational force/acceleration

$$\vec{a}_G(r, \theta) = \int_{r'} \int_{\theta'} \frac{-\sigma(r', \theta') r' dr' d\theta'}{(r^2 + r'^2 - 2rr' \cos(\theta - \theta'))^{\frac{3}{2}}} \begin{pmatrix} r - r' \cos(\theta - \theta') \\ r' \sin(\theta - \theta') \end{pmatrix}$$

- things to be learned:
 - ▶ Fortran
 - ▶ General programming experience
 - ▶ Code optimization
 - ▶ Balancing speed vs. accuracy
- issues:
 - ▶ Time
 - ▶ Boundary conditions
 - ▶ Numerical stability

First Program

- most accurate calculation on level 0 as a reference
 - ▶ Open files
 - ▶ Read data into arrays
 - ▶ Loop through all grid points (i,j) (force)
 - ▶ Nested loop through all grid centres (i',j') (density)
 - ▶ Calculate formula inside inner loop
 - ▶ Write force into new file
- other versions (higher levels) have similar structure

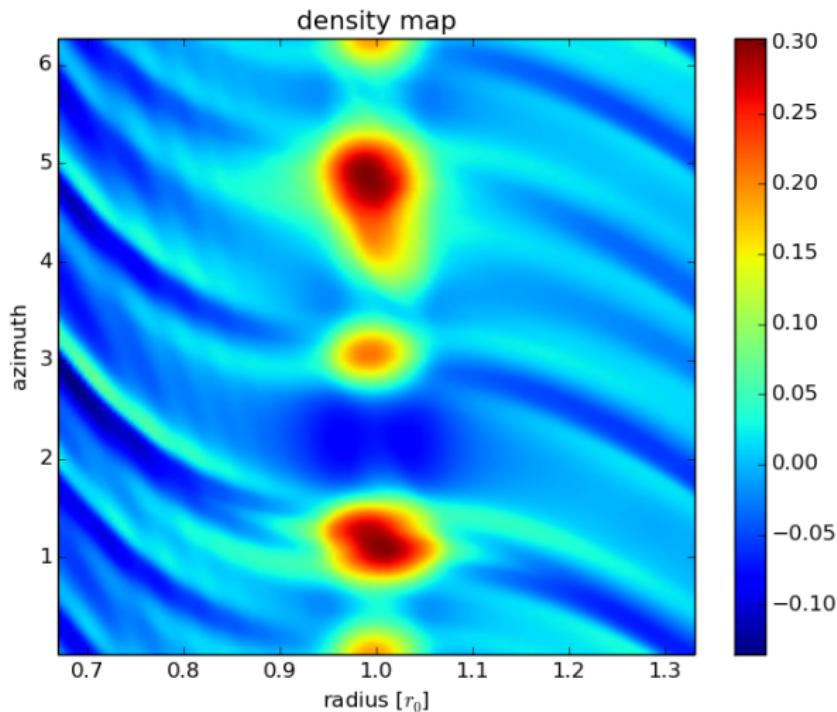
Simple Implementation

```
! write force components for every corner in grid
do i = 1, N_r
    r_i = r(i)-.5*dr(i) ! shift r to the corners
    do j = 1, N_theta
        theta_j = theta(j)-.5*dtheta(j) ! shift theta to the corners
        ! sum up the forces onto the point (i, j)
        do iprime = 1, N_r
            do jprime = 1, N_theta
                force_point = -sigma(iprime,jprime)*r(iprime)*dr(iprime)*dtheta(jprime)/(r_i**2+r(iprime)**2-2.*r_i*r(iprime)*cos(theta_j-theta(jprime)))**1.5
                f_r = f_r + force_point * (r_i-r(iprime))*cos(theta_j-theta(jprime))
                f_theta = f_theta + force_point * r(iprime)*sin(theta_j-theta(jprime))
            end do
        end do
        write(11, '(e20.10)') f_r
        write(12, '(e20.10)') f_theta
        f_r = 0.
        f_theta = 0.
    end do
end do
```

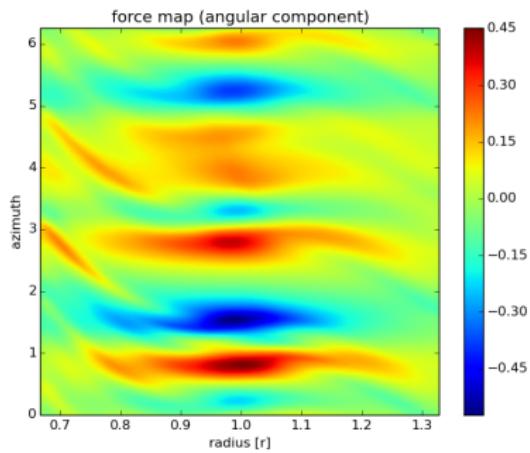
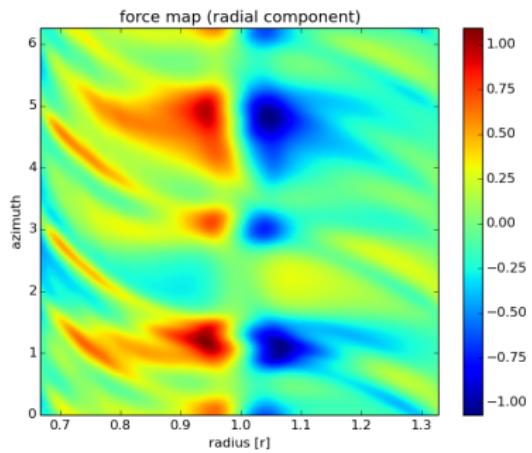
Optimization Strategies

- Fortran loops are column-major (todo:arrays?)
- minimizing loop overhead:
 - ▶ Avoid subroutine calls in inner loops
 - ▶ Reduce repeat evalutions by shifting to outer loops
- Loop unrolling (if compiler optimization doesn't already do it)
- Faster arithmetic operations, e.g. $a*a$ instead of $a**2$ (multiplications instead of exponentials and logarithms)
- Idea: find faster methods, e.g. `invsqrt` using bit shifts and Newton iterations (additions and multiplications instead of divisions)
- Precalculations of lookup tables for grid given parameters (`cos`, `sin`, `r_prime`, `theta_prime` etc.)
- Using symmetries
 - time optimization from 255.95s to 9.87 s (v. 1)
 - time optimization from 69.0s to 11.8 s (v. 2)

Density map

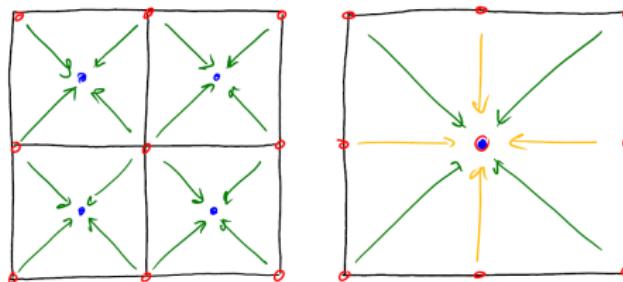


Level 0



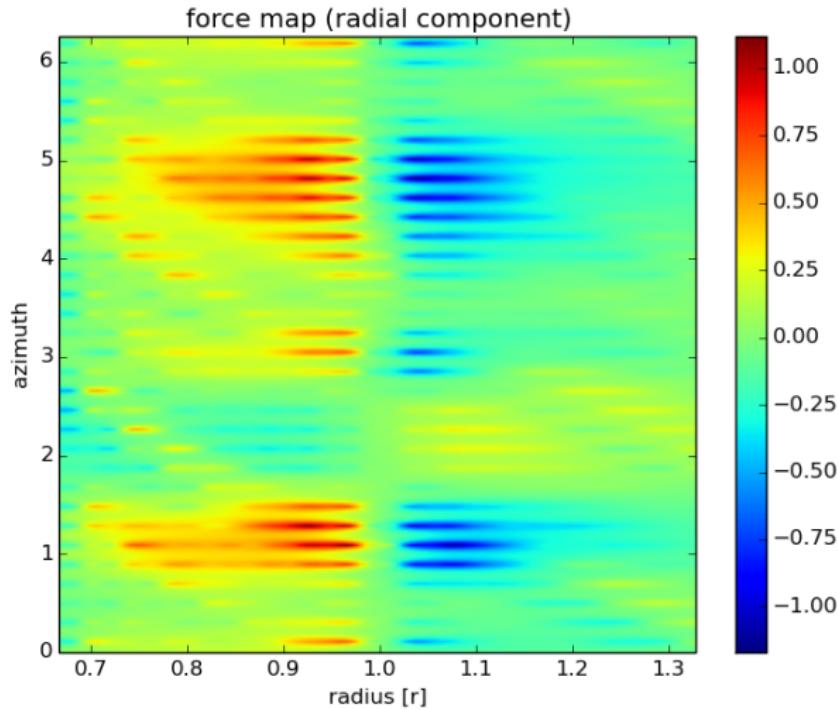
Higher levels

- Reducing operations by using fewer mass points
- 4^{LEVEL} cells into 1
- Problem: oscillations
- Cause: calculation not anymore only at corners of the grid cells
- First solution:
 - ▶ shift to corner
 - ▶ interpolate the masses
 - ▶ introduce ghost cells



point of calculation
position of mass point
distance from a corner
distance from a non-corner point

Oscillation pattern (TODO: Level 3?)



Bilinear interpolation

for unit square:

$$f(x, y) \approx f(0, 0)(1-x)(1-y) + f(1, 0)x(1-y) + f(0, 1)(1-x)y + f(1, 1)xy$$

$$f(\alpha, \beta) \approx f(0, 0)(1-\alpha)(1-\beta) + f(1, 0)\alpha(1-\beta) + f(0, 1)(1-\alpha)\beta + f(1, 1)\alpha\beta$$

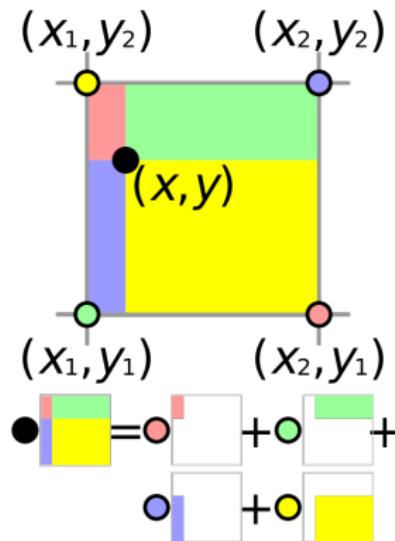
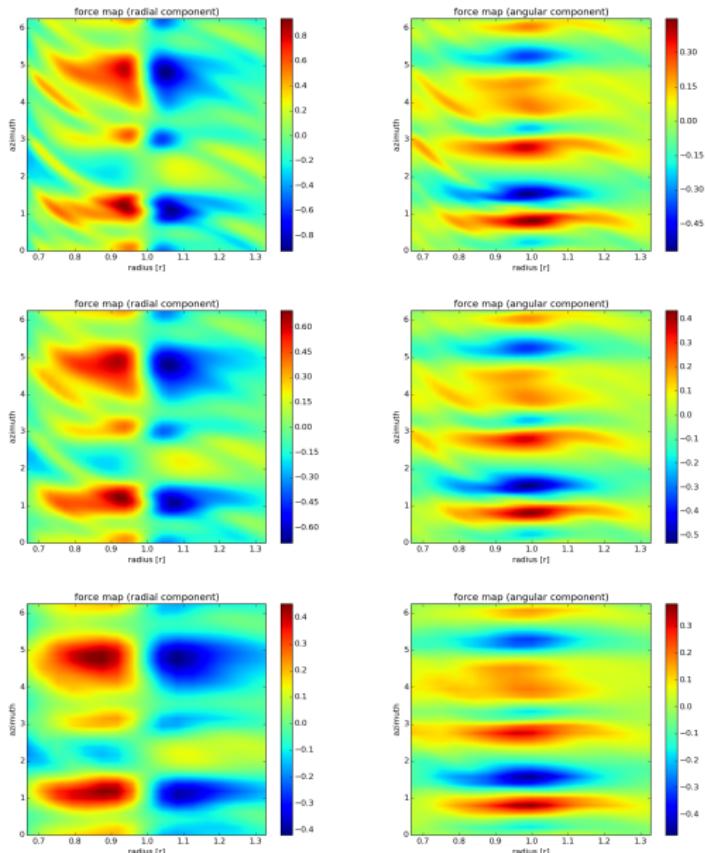


Figure : http://upload.wikimedia.org/wikipedia/commons/9/91/7_Bilinear_interpolation_visualisation.svg

Pure Levels 1, 2 and 3



Refinement with a single level

- task: calculate level 3 grid with refinement from level 2
- closest 4 by 4 cells calculated with one level below
- problem: periodic boundary conditions

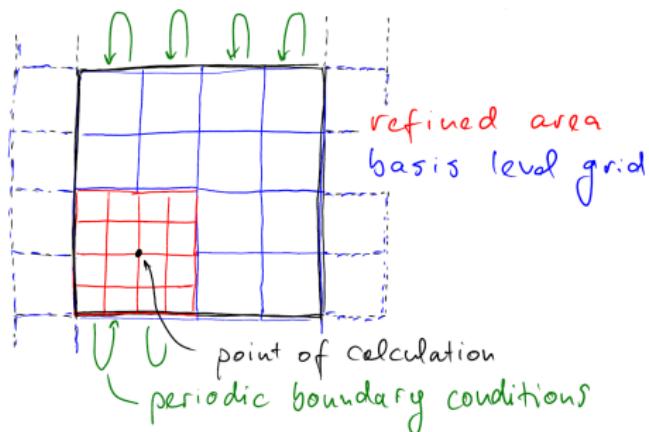


Figure : sketch by Philipp Denzel

Code

```
do i = 1, N_r0
    r_corner = r0(i)-.5*dr0(i)
    do j = 1, N_theta0
        theta_corner = theta0(j)-.5*dtheta0(j)
        call shift_param ! gives shifts: ishift(ref), jshift(ref), dr_shift(ref), dtheta_shift(ref)
        call ref_area ! gives refined area boundaries: iref_low/up, ix_low/up, periodic_low/up
        call intrpltn_coeff ! gives coefficients: c1, c2, c3, c4, ciref, c2ref, c3ref, c4ref
        do iprime = iref_low, iref_up
            do jprime = jref_low, jref_up
                ...end do
            end do
        do iprime = 0, ix_low-1
            do jprime = 1, N_thetax
                ...end do
            end do
        do iprime = ix_up+1, N_rx
            do jprime = 1, N_thetax
                ...end do
            end do
        do iprime = ix_low, ix_up
            do jprime = 1+periodic_up, jx_low-1
                ...end do
            end do
        do iprime = ix_low, ix_up
            do jprime = jx_up+1, N_thetax-periodic_low
                ...end do
            end do
        end do
    end do
end do
```

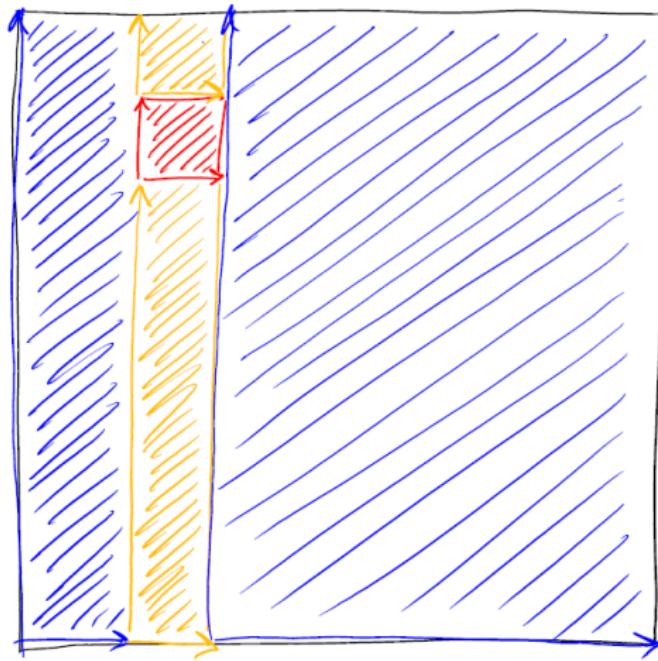
Inner loop calculation

```
vmass = ( c1 * masssx(iprime, jprime) + c2 * masssx(iprime+1, jprime) +&
          &c3 * masssx(iprime, jprime+1)+ c4 * masssx(iprime+1, jprime+1))&
          & * inv_factor2
! calculate shifted values
rprime = rx(iprime)+dr_shift
ratio = r_corner/rprime
delta_theta = theta_corner-thetax(jprime)-dtheta_shift
cosine = cos(delta_theta)
denom_point = 1.+ratio*ratio-2.*ratio*cosine
denom_point = sqrt(denom_point)*denom_point*rprime*rprime
force_point = vmass/denom_point
force_r(i,j) = force_r(i,j)+force_point*(ratio-cosine)
force_theta(i,j) = force_theta(i,j)+force_point*sin(delta_theta)
```

or for the refined area...

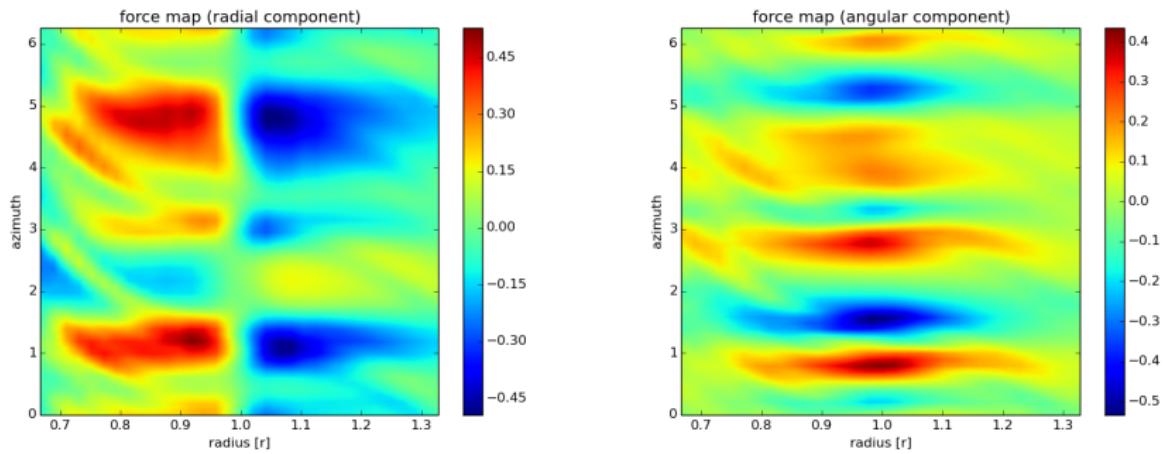
```
vmass = ( c1ref * massxref(iprime, jprime) + c2ref * massxref(iprime+1, jprime) +&
          &c3ref * massx(iprime, jprime+1) + c4ref * massxref(iprime+1, jprime+1))&
          & * inv_factor2ref
! calculate shifted values
rprime = rxref(iprime)+dr_shiftref
ratio = r_corner/rprime
delta_theta = theta_corner-thetaxref(jprime)-dtheta_shiftrref
cosine = cos(delta_theta)
denom_point = 1.+ratio*ratio-2.*ratio*cosine
denom_point = sqrt(denom_point)*denom_point*rprime*rprime
force_point = vmass/denom_point
force_r(i,j) = force_r(i,j)+force_point*(ratio-cosine)
force_theta(i,j) = force_theta(i,j)+force_point*sin(delta_theta)
```

Schematics

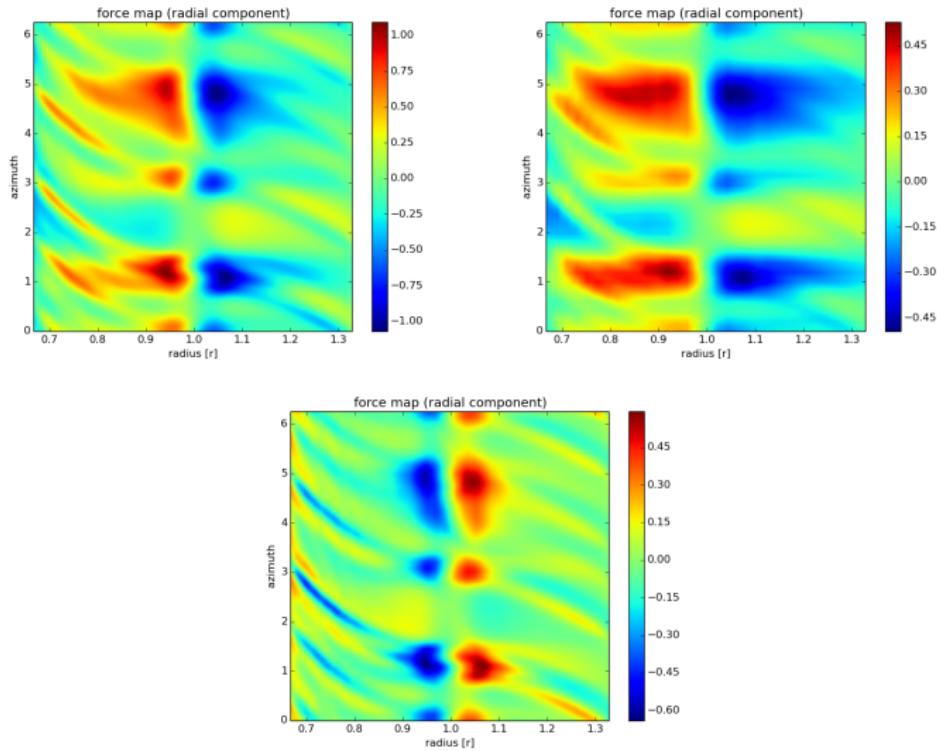


refined area
areas left
and right
areas below
and above

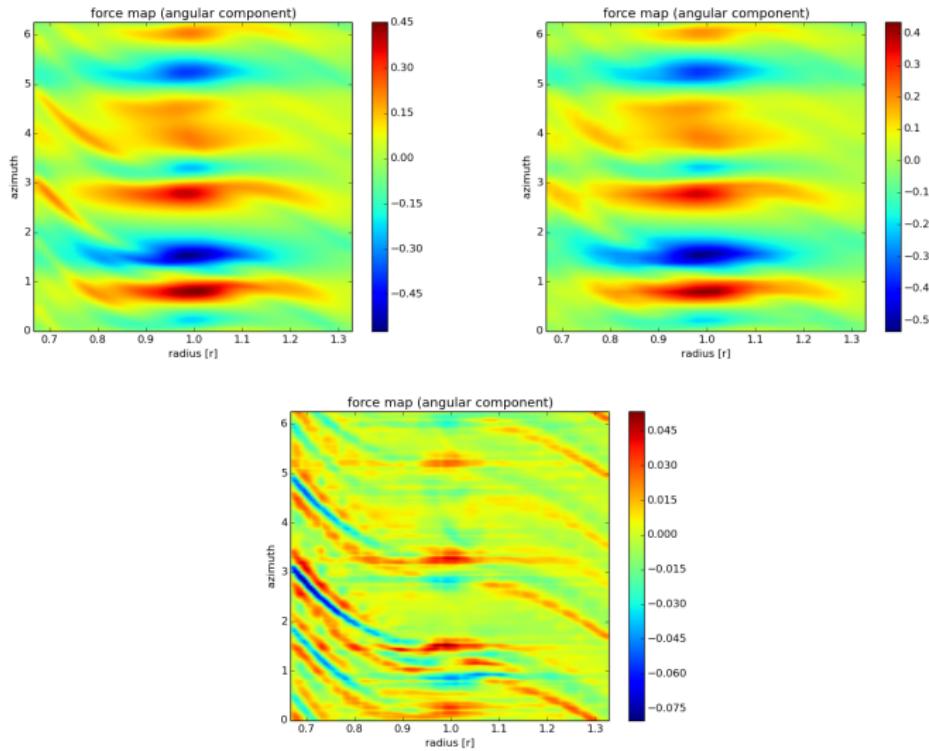
Results - Level 3 with refinement



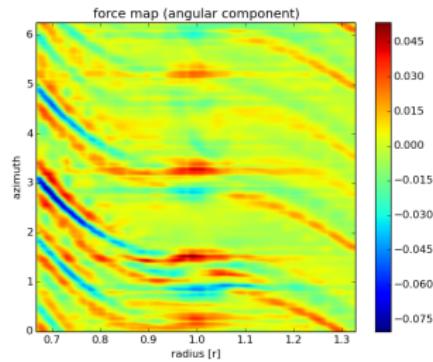
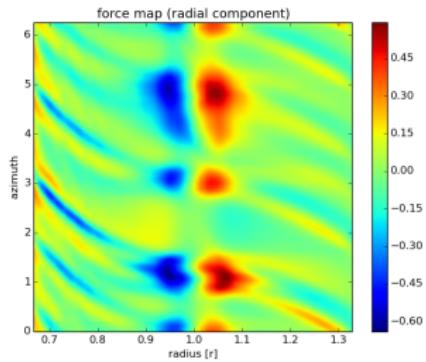
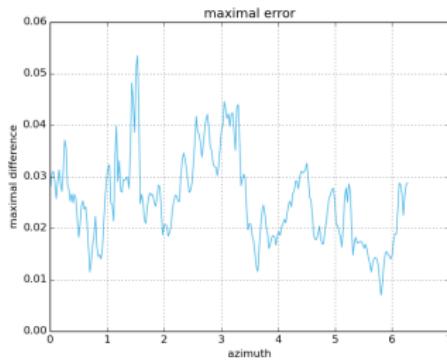
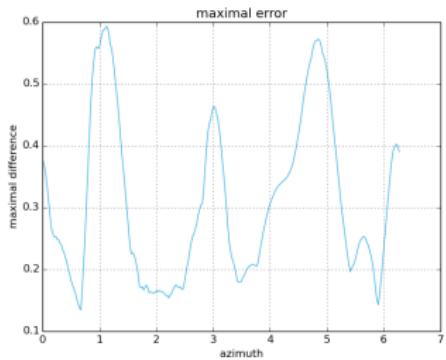
Differences to Level 0 - radial component



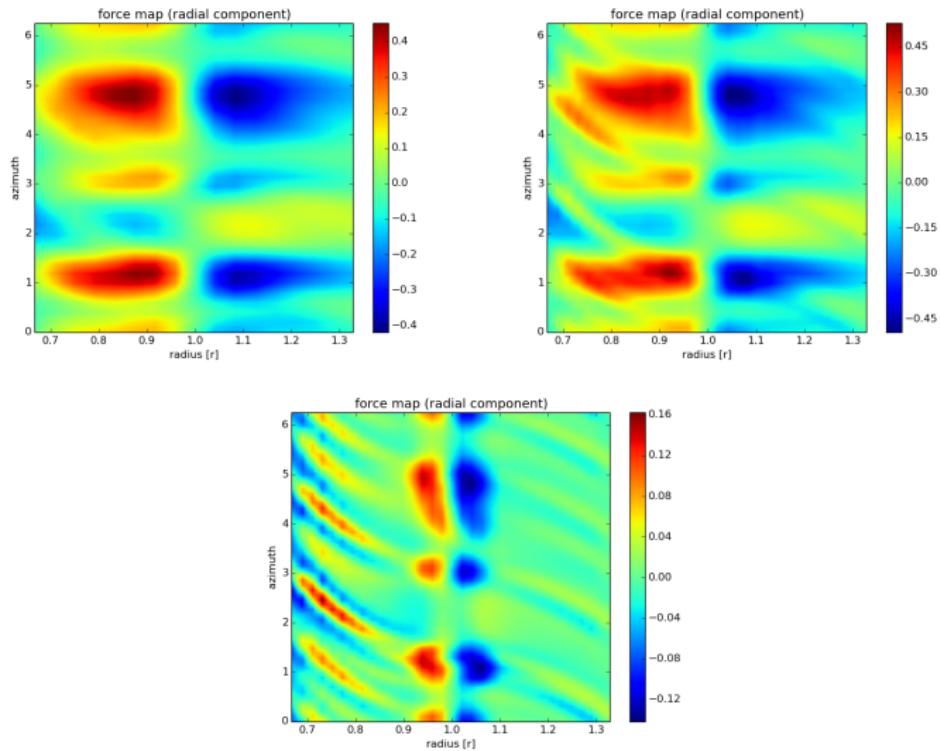
Differences to Level 0 - angular component



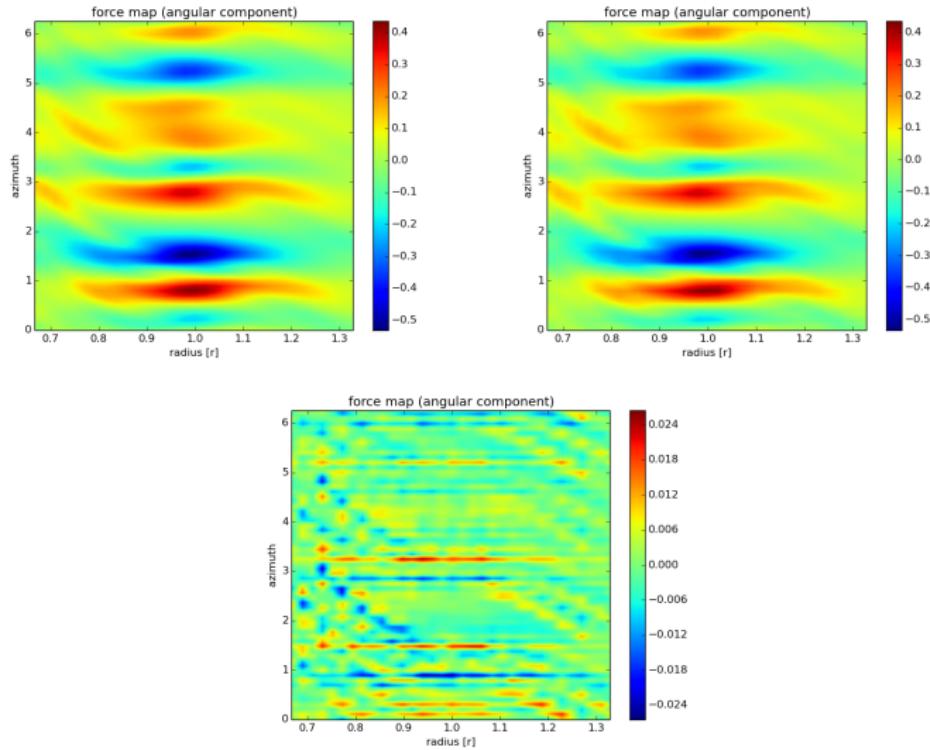
Maximal difference in a row



Improvement by refinement - radial component

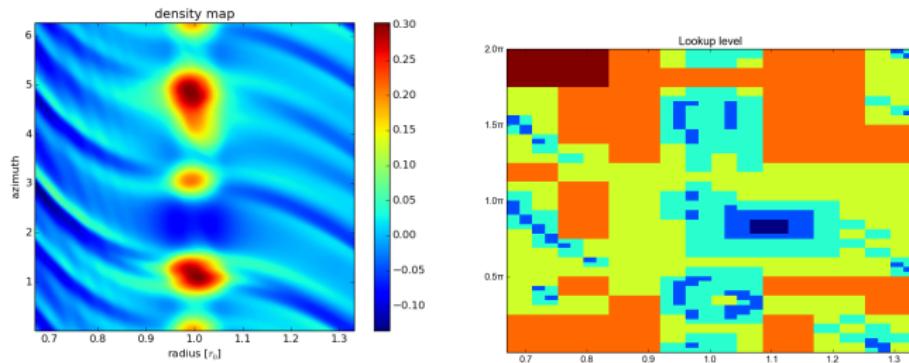


Comparison to Level 2 - angular component



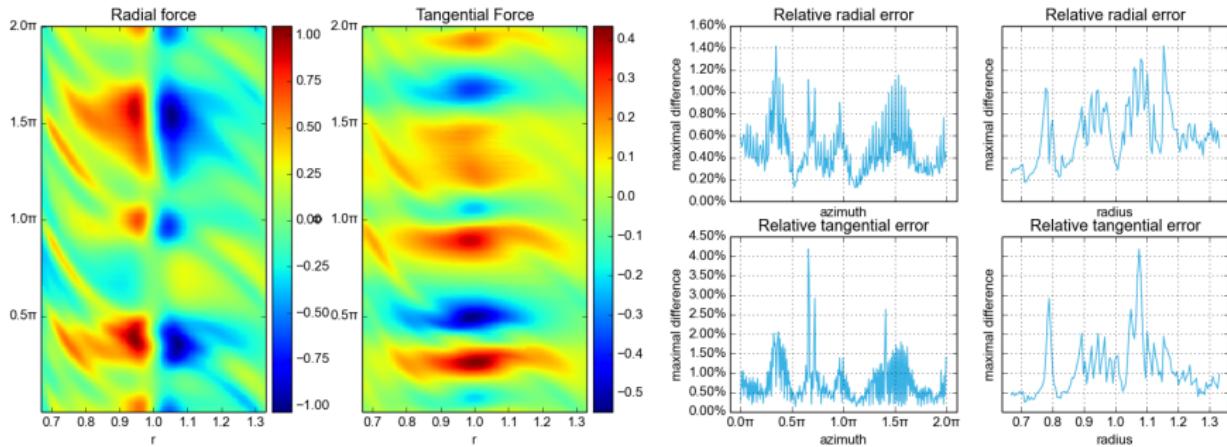
How can we improve this?

- Adaptive lookup down to level 0; Based on:
 - ▶ Distance
 - ▶ Magnitude of difference in mass of lower level cells



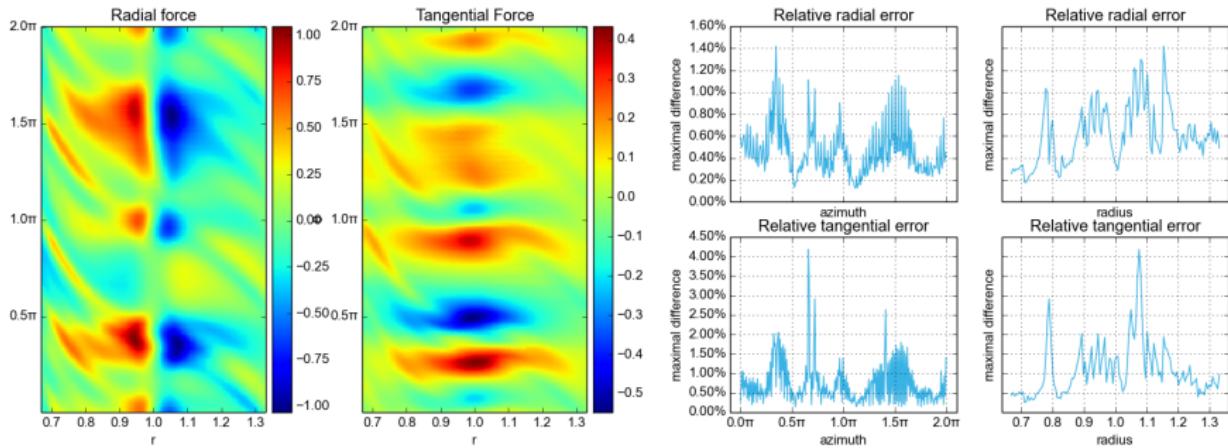
Result

- Simulation time: approx. 4s
- Error bound: less than 4.5 percent at peaks
- Oscillation patterns still exist



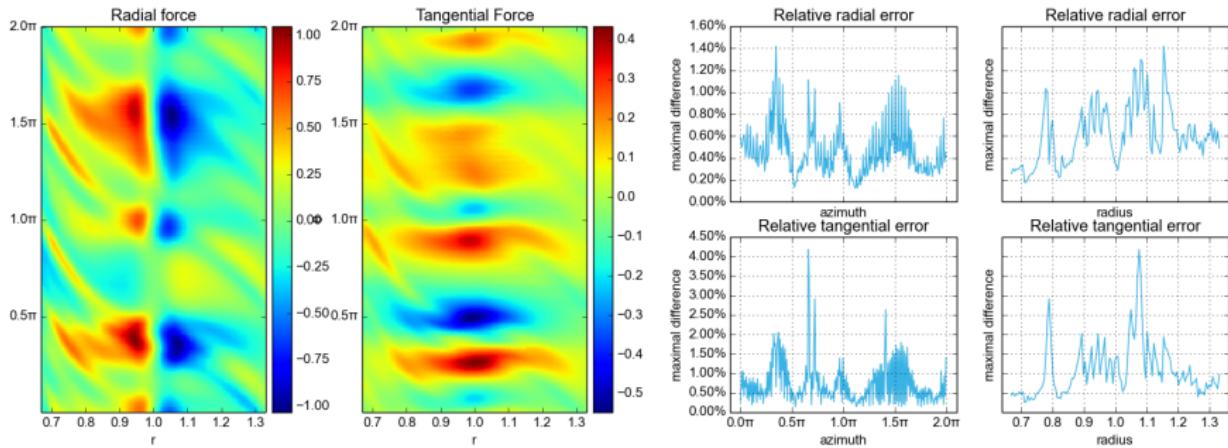
More about adaptive Code - 1

- item1
- item2
- item3



More about adaptive Code - 2

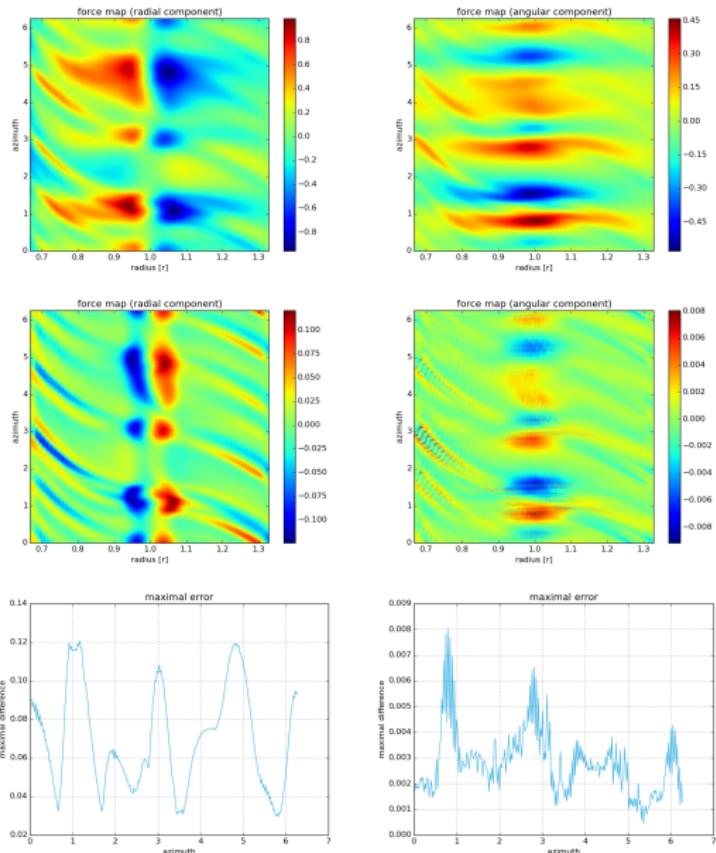
- item1
- item2
- item3



Thanks for listening!

Questions?

Results for Level 1 with refinement



InvSqrt

http://en.wikipedia.org/wiki/Fast_inverse_square_root

Custom InvSqrt

```
REAL(8) FUNCTION InvSqrt (x)
IMPLICIT NONE
TYPE casting
    REAL(8) :: x
END TYPE casting
REAL(8), INTENT(in) :: x
! casting
TYPE(casting), TARGET :: pointerTo
! Encode data as an array of integers
INTEGER(8), DIMENSION(:), ALLOCATABLE :: enc
INTEGER(8) :: length
INTEGER(8) :: magic_number = 6910469410427058089
REAL(8) :: xhalf
xhalf = .5*x
! transfer to heap
pointerTo%x = x
! encode a memory section from a type to other
length = size(transfer(pointerTo, enc))
allocate(enc(length))
! encoded to integer
enc = transfer(pointerTo, enc) ! evil floating point bit level hacking
enc(1) = magic_number - rshift(enc(1),1) ! wtf! (for int64: 0x5fe6eb50c7b537a9 = 6910469410427058089)
! decode
pointerTo = transfer(enc, pointerTo)
! dealloc
deallocate(enc)

InvSqrt = pointerTo%x*(1.5 - xhalf*pointerTo%x*pointerTo%x)
END FUNCTION InvSqrt
```