



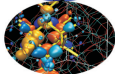
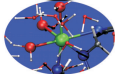
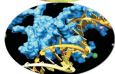
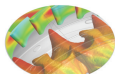
OpenMP Exercises

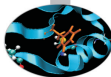
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Cristiano Padrin - c.padrin@cineca.it

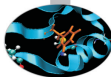
SuperComputing Applications and Innovation Department





Warm-up with OpenMP

- 1 Compile and run "Hello World" and experiment with the `OMP_NUM_THREADS` variable. If any errors occur, try to fix it.
- 2 Parallelize the MM (Matrix Multiplication) serial code acting only on the most important loop



Warm-up with OpenMP

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- 2 Parallelize the MM (Matrix Multiplication) serial code acting only on the most important loop



Hello World from C

C

```
#include <stdio.h>
#ifdef _OPENMP
#include<omp.h>
#endif
int main(int argc, char* argv[ ])
{
#ifdef _OPENMP
    int iam;
    #pragma omp parallel /* the parallel block starts here */
    {
        iam=omp_get_thread_num();

        #pragma omp critical
        printf("Hello from %d\n",iam);

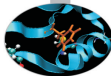
    } /* the parallel block ends here */
#else
    printf("Hello, this is a serial program.\n");
#endif
    return 0;
}
```



Hello World from Fortran

Fortran

```
Program Hello_from_Threads
#ifdef _OPENMP
  use omp_lib
#endif
  implicit none
  integer :: iam
#ifdef _OPENMP
  !$omp parallel
    iam=omp_get_thread_num()
    !$omp critical
      write( *,* ) 'Hello from', iam
    !$omp end critical
  !$omp end parallel
#else
  write( *,* ) 'Hello, this is a serial program'
#endif
end program Hello_from_Threads
```



Hello World from C

C

```
#include <stdio.h>
#ifdef _OPENMP
#include<omp.h>
#endif
int main(int argc, char* argv[ ])
{
#ifdef _OPENMP
    int iam;
    #pragma omp parallel \
private(iam) /* the parallel block starts here */
    {
        iam=omp_get_thread_num();

        #pragma omp critical
        printf("Hello from %d\n",iam);

    } /* the parallel block ends here */
#else
    printf("Hello, this is a serial program.\n");
#endif
    return 0;
}
```



Hello World from Fortran

Fortran

```
Program Hello_from_Threads
#ifdef _OPENMP
  use omp_lib
#endif
  implicit none
  integer :: iam
#ifdef _OPENMP
  !$omp parallel &
  !$omp private(iam)
    iam=omp_get_thread_num()
    !$omp critical
      write( *,* ) 'Hello from', iam
    !$omp end critical
  !$omp end parallel
#else
  write( *,* ) 'Hello, this is a serial program'
#endif
end program Hello_from_Threads
```



Warm-up with OpenMP

- 1 Compile and run "Hello World" and experiment with the `OMP_NUM_THREADS` variable. If any errors occur, try to fix it.
- 2 Parallelize the MM (Matrix Multiplication) serial code acting only on the most important loop



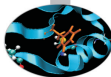
Matrix Multiplication in C

```
C
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

int main(int argc, char **argv) {
    int n;
    int i, j, k;
    ...
    double ( *a ) [n] = malloc(sizeof(double[n] [n]));
    double ( *b ) [n] = malloc(sizeof(double[n] [n]));
    double ( *c ) [n] = malloc(sizeof(double[n] [n]));
    ...

    for (i=0; i<n; i++)
        for (j=0; j<n; j++) {
            a[i][j] = ((double) rand())/((double) RAND_MAX);
            b[i][j] = ((double) rand())/((double) RAND_MAX);
            c[i][j] = 0.0;
        }

    for (i=0; i<n; ++i)
        for (k=0; k<n; k++)
            for (j=0; j<n; ++j)
                c[i][j] += a[i][k]*b[k][j];
    ...
    return 0;
}
```



Matrix Multiplication in Fortran

Fortran

```
program mat_prod
  implicit none
  integer :: n
  real(kind(1.d0)), dimension(:,,:), allocatable :: a, b, c
  integer :: i, j, k
  ...
  allocate(a(n,n),b(n,n),c(n,n),stat=ierr)
  ...
  call random_number(a)
  call random_number(b)
  c = 0.d0

  do j=1, n
    do k=1, n
      do i=1, n
        c(i,j) = c(i,j) + a(i,k)*b(k,j)
      end do
    end do
  end do

  ...
end program mat_prod
```



Matrix Multiplication in C

```
C
#include <stdio.h>
#include <stdlib.h>
#include <math.h>

int main(int argc, char **argv) {
    int n;
    int i, j, k;
    ...
    double ( *a ) [n] = malloc(sizeof(double[n] [n]));
    double ( *b ) [n] = malloc(sizeof(double[n] [n]));
    double ( *c ) [n] = malloc(sizeof(double[n] [n]));
    ...

    for (i=0; i<n; i++)
        for (j=0; j<n; j++) {
            a[i][j] = ((double) rand())/((double) RAND_MAX);
            b[i][j] = ((double) rand())/((double) RAND_MAX);
            c[i][j] = 0.0;
        }

    #pragma omp parallel for private(j,k)
        for (i=0; i<n; ++i)
            for (k=0; k<n; k++)
                for (j=0; j<n; ++j)
                    c[i][j] += a[i][k]*b[k][j];
    ...
    return 0;
}
```

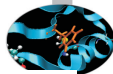


Matrix Multiplication in Fortran

Fortran

```
program mat_prod
  implicit none
  integer :: n
  real(kind(1.d0)), dimension(:,,:), allocatable :: a, b, c
  integer :: i, j, k
  ...
  allocate(a(n,n),b(n,n),c(n,n),stat=ierr)
  ...
  call random_number(a)
  call random_number(b)
  c = 0.d0

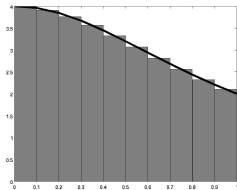
  !$omp parallel do
    do j=1, n
      do k=1, n
        do i=1, n
          c(i,j) = c(i,j) + a(i,k)*b(k,j)
        end do
      end do
    end do
  !$omp end parallel do
  ...
end program mat_prod
```



Let's play with OpenMP

- 3 Parallelize the serial code `Pi`. It computes the Reimann approximation of

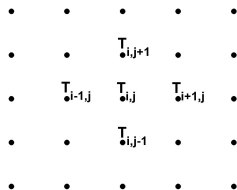
$$\int_0^1 \frac{4}{1+x^2} dx = 4 \arctan x \Big|_0^1 = \pi$$

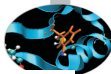


- 4 Parallelize the serial code `Laplace`. It applies the iterative Jacobi method to a finite differences approximation of the Laplace equation with Dirichlet boundary condition:

$$T_{i,j}^{n+1} = \frac{1}{4}(T_{i+1,j}^n + T_{i-1,j}^n + T_{i,j-1}^n + T_{i,j+1}^n)$$

- start from the most computationally intensive loop
- then try to include the `while` loop in the parallel region

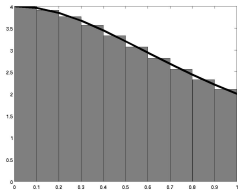




Let's play with OpenMP

- 3 Parallelize the serial code `Pi`. It computes the Reimann approximation of

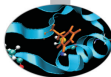
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$$T_{i,j}^{n+1} = \frac{1}{4}(T_{i+1,j}^n + T_{i-1,j}^n + T_{i,j-1}^n + T_{i,j+1}^n)$$

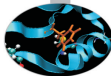
- start from the most computationally intensive loop
- then try to include the `while` loop in the parallel region



π

C

```
...  
  
sum = 0.0;  
dx = 1.0 / (double) intervals;  
  
for (i = 1; i <= n; i++) {  
    x = dx * ((double) (i - 0.5));  
    f = 4.0 / (1.0 + x*x);  
    sum = sum + f;  
}  
pi = dx*sum;  
  
...
```



Fortran

...

```
sum=0.d0
```

```
dx=1.d0/intervals
```

```
do i=1,n
```

```
  x=dx*(i-0.5d0)
```

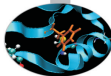
```
  f=4.d0/(1.d0+x*x)
```

```
  sum=sum+f
```

```
end do
```

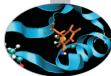
```
pi=dx*sum
```

...



C

```
#include <omp.h>
...
double timel = omp_get_wtime();
sum = 0.0;
dx = 1.0 / (double) intervals;
#pragma omp parallel for private(x,f) reduction(+:sum)
for (i = 1; i <= n; i++) {
    x = dx * ((double) (i - 0.5));
    f = 4.0 / (1.0 + x*x);
    sum = sum + f;
}
pi = dx*sum;
time2 = omp_get_wtime() - timel;
...
```



Fortran

```
use omp_lib
...
time1 = omp_get_wtime()
sum=0.d0
dx=1.d0/intervals
!$omp parallel do private(x,f) reduction(+:sum)
do i=1,n
  x=dx*(i-0.5d0)
  f=4.d0/(1.d0+x*x)
  sum=sum+f
end do
!$omp end parallel do
pi=dx*sum
time2 = omp_get_wtime()
...
```



Let's play with OpenMP

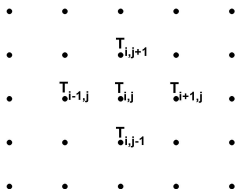
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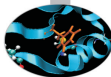
$$\int_0^1 \frac{4}{1+x^2} dx = 4 \arctan x \Big|_0^1 = \pi$$

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$$T_{i,j}^{n+1} = \frac{1}{4} (T_{i+1,j}^n + T_{i-1,j}^n + T_{i,j-1}^n + T_{i,j+1}^n)$$

- start from the most computationally intensive loop
- then try to include the `while` loop in the parallel region





Laplace

```
C
...
while(var > tol && iter <= maxIter) {
    ++iter;
    var = 0.0;

    for (i=1; i<=n; ++i)
        for (j=1; j<=n; ++j) {
            Tnew[i*n2+j] = 0.25*(T[(i-1)*n2+j] + T[(i+1)*n2+j]
                                + T[i*n2+(j-1)] + T[i*n2+(j+1)]);
            var = fmax(var, fabs(Tnew[i*n2+j] - T[i*n2+j]));
        }
    Tmp=T; T=Tnew; Tnew=Tmp;
    if (iter%100 == 0)
        printf("iter: %8u, variation = %12.4lE\n", iter, var);
}
...
```

Laplace



Fortran

```
...  
do while (var > tol .and. iter <= maxIter)  
  iter = iter + 1  
  var = 0.d0  
  
  do j = 1, n  
    do i = 1, n  
      Tnew(i,j)=0.25d0*(T(i-1,j)+T(i+1,j)+T(i,j-1)+T(i,j+1))  
      var = max(var, abs( Tnew(i,j) - T(i,j) ))  
    end do  
  end do  
  
  Tmp =>T; T =>Tnew; Tnew => Tmp;  
  if( mod(iter,100) == 0 ) ...  
end do  
...
```

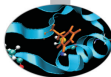


Laplace

```

C
...
while(var > tol && iter <= maxIter) {
  ++iter;
  var = 0.0;
  #pragma omp parallel for private(j) reduction(max:var)
  for (i=1; i<=n; ++i)
    for (j=1; j<=n; ++j) {
      Tnew[i*n2+j] = 0.25*(T[(i-1)*n2+j] + T[(i+1)*n2+j]
                          + T[i*n2+(j-1)] + T[i*n2+(j+1)]);
      var = fmax(var, fabs(Tnew[i*n2+j] - T[i*n2+j]));
    }
  Tmp=T; T=Tnew; Tnew=Tmp;
  if (iter%100 == 0)
    printf("iter: %8u, variation = %12.4lE\n", iter, var);
}
...

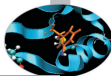
```



Laplace

Fortran

```
...  
do while (var > tol .and. iter <= maxIter)  
  iter = iter + 1  
  var = 0.d0  
  !$omp parallel do reduction(max:var)  
  do j = 1, n  
    do i = 1, n  
      Tnew(i,j)=0.25d0*(T(i-1,j)+T(i+1,j)+T(i,j-1)+T(i,j+1))  
      var = max(var, abs( Tnew(i,j) - T(i,j) ))  
    end do  
  end do  
  !$omp end parallel do  
  Tmp =>T; T =>Tnew; Tnew => Tmp;  
  if( mod(iter,100) == 0 ) ...  
end do  
...
```



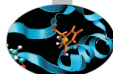
Lacks support for OpenMP 3.1?

C

```
while(var > tol && iter <= maxIter) {
    ++iter;
    var = 0.0;

    for (i=1; i<=n; ++i)
        for (j=1; j<=n; ++j) {
            Tnew[i*n2+j] = 0.25*( T[(i-1)*n2+j] + T[(i+1)*n2+j]
                                + T[i*n2+(j-1)] + T[i*n2+(j+1)] );
            var = fmax(var , fabs(Tnew[i*n2+j] - T[i*n2+j]));
        }

    }
    Tmp=T; T=Tnew; Tnew=Tmp;
    if (iter%100 == 0) ...
}
```

Lacks support for OpenMP 3.1?

C

```

while(var > tol && iter <= maxIter) {
  ++iter;
  var = 0.0;
  #pragma omp parallel
  {
    double pvar = 0.0;
    #pragma omp for private(j)
    for (i=1; i<=n; ++i)
      for (j=1; j<=n; ++j) {
        Tnew[i*n2+j] = 0.25*( T[(i-1)*n2+j] + T[(i+1)*n2+j]
                               + T[i*n2+(j-1)] + T[i*n2+(j+1)] );
        pvar = fmax(pvar , fabs(Tnew[i*n2+j] - T[i*n2+j]));
      }
    #pragma omp critical
    if (pvar > var) var = pvar;
  }
  Tmp=T; T=Tnew; Tnew=Tmp;
  if (iter%100 == 0) ...
}
  
```



Let's play with OpenMP

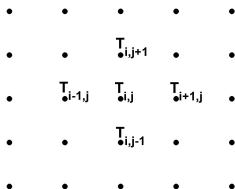
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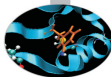
$$\int_0^1 \frac{4}{1+x^2} dx = 4 \arctan x \Big|_0^1 = \pi$$

- 4 Parallelize the serial code `Laplace`. It applies the iterative Jacobi method to a finite differences approximation of the Laplace equation with Dirichlet boundary condition:

$$T_{i,j}^{n+1} = \frac{1}{4}(T_{i+1,j}^n + T_{i-1,j}^n + T_{i,j-1}^n + T_{i,j+1}^n)$$

- start from the most computationally intensive loop
- then try to include the **while** loop in the parallel region

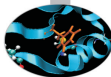




Laplace incremented

C

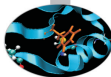
```
...  
  
while(var > tol && iter <= maxIter) {  
  
    ++iter;  
    var = 0.0;  
  
    #pragma omp for private(j) reduction(max:var)  
    ...  
  
    Tmp=T; T=Tnew; Tnew=Tmp;  
    if (iter%100 == 0) ...  
  
}  
  
...
```



Laplace incremented

Fortran

```
...  
  
do while (var > tol .and. iter <= maxIter)  
  
    iter = iter + 1  
    var = 0.d0  
  
    !$omp do reduction(max:var)  
    ...  
    !$omp end do  
  
    Tmp =>T; T =>Tnew; Tnew => Tmp;  
    if( mod(iter,100) == 0 ) ...  
  
end do  
  
...
```



Laplace incremented

C

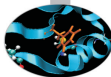
```
...
#pragma omp parallel
{
    while(var > tol && iter <= maxIter) {

        ++iter;
        var = 0.0;

        #pragma omp for private(j) reduction(max:var)
        ...

        Tmp=T; T=Tnew; Tnew=Tmp;
        if (iter%100 == 0) ...

    }
}
...
```



Laplace incremented

C

```
...
#pragma omp parallel
{
    while(var > tol && iter <= maxIter) {

        #pragma omp single
        {
            ++iter;
            var = 0.0;
        }
        #pragma omp for private(j) reduction(max:var)
        ...
        #pragma omp single
        {
            Tmp=T; T=Tnew; Tnew=Tmp;
            if (iter%100 == 0) ...
        }
    }
}
...
```



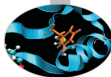
Laplace incremented

C

```
...
#pragma omp parallel
{
  while(var > tol && iter <= maxIter) {
    #pragma omp barrier
    #pragma omp single
    {
      ++iter;
      var = 0.0;

      #pragma omp for private(j) reduction(max:var)
      ...
      #pragma omp single nowait
      {
        Tmp=T; T=Tnew; Tnew=Tmp;
        if (iter%100 == 0) ...
      }
    }
  }
}
...

```



Laplace incremented

Fortran

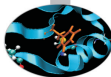
```
...
!$omp parallel
  do while (var > tol .and. iter <= maxIter)

    iter = iter + 1
    var = 0.d0

    !$omp do reduction(max:var)
      ...
    !$omp end do

    Tmp =>T; T =>Tnew; Tnew => Tmp;
    if( mod(iter,100) == 0 ) ...

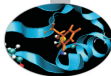
  end do
!$omp end parallel
...
```

Laplace incremented

Fortran

```
...  
!$omp parallel  
  do while (var > tol .and. iter <= maxIter)  
  
    !$omp single  
      iter = iter + 1  
      var = 0.d0  
    !$omp end single  
    !$omp do reduction(max:var)  
      ...  
    !$omp end do  
    !$omp single  
      Tmp =>T; T =>Tnew; Tnew => Tmp;  
      if( mod(iter,100) == 0 ) ...  
    !$omp end single  
  end do  
!$omp end parallel  
...
```



Laplace incremented

Fortran

```
...  
!$omp parallel  
do while (var > tol .and. iter <= maxIter)  
  !$omp barrier  
  !$omp single  
    iter = iter + 1  
    var = 0.d0  
  !$omp end single  
  !$omp do reduction(max:var)  
    ...  
  !$omp end do  
  !$omp single  
    Tmp =>T; T =>Tnew; Tnew => Tmp;  
    if( mod(iter,100) == 0 ) ...  
  !$omp end single nowait  
end do  
!$omp end parallel  
...
```



Still lacks OpenMP 3.1 support?

```

C
#pragma omp parallel
{
  while(var > tol && iter <= maxIter) {
    #pragma omp barrier
    #pragma omp single
    {
      ++iter;
      var = 0.0;
    }
    double pvar = 0.0;
    #pragma omp for nowait private(j)
    for (i=1; i<=n; ++i)
      for (j=1; j<=n; ++j) {
        Tnew[i*n2+j] = 0.25*( T[(i-1)*n2+j] + T[(i+1)*n2+j]
                             + T[i*n2+(j-1)] + T[i*n2+(j+1)] );
        pvar = fmax(pvar, fabs(Tnew[i*n2+j] - T[i*n2+j]));
      }
    #pragma omp critical
    if (pvar > var) var = pvar;

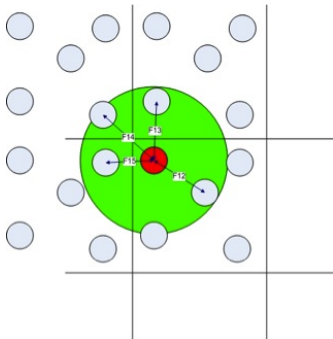
    #pragma omp barrier
    #pragma omp single nowait
    {
      Tmp=T; T=Tnew; Tnew=Tmp;
      if (iter%100 == 0) printf("iter: %8u, variation = %12.41E\n", iter, var);
    }
  }
}
  
```



When the Going Gets Tough, ...

5 Parallelize the serial code **Nbody**. It computes the total energy and the forces of a system of N particles with potential $V = 1/r$ if r is less of a threshold and $V = 0$ otherwise.

- pay attention to the update of **forces**
 - try to update them atomically
 - try to reduce them
 - try different schedules and test their performance
-
- to compile use the preprocessing MACRO DIM=55000, for example
 - `gcc -O3 -DDIM=55000 Nbody.c -o nbody -lm`

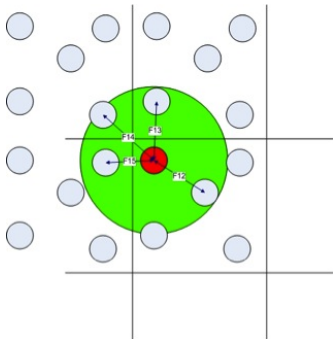




When the Going Gets Tough, ...

5 Parallelize the serial code **Nbody**. It computes the total energy and the forces of a system of N particles with potential $V = 1/r$ if r is less of a threshold and $V = 0$ otherwise.

- pay attention to the update of **forces**
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-
- to compile use the preprocessing MACRO DIM=55000, for example
 - `gcc -O3 -DDIM=55000 Nbody.c -o nbody -lm`



Nbody

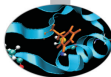


C

```
for(i=0; i<nbodies; ++i)
  for(j=i+1; j<nbodies; ++j) {
    d2 = 0.0;
    for(k=0; k<3; ++k) {
      rij[k] = pos[i][k] - pos[j][k];
      d2 += rij[k]*rij[k];
    }
    if (d2 <= cut2) {
      d = sqrt(d2);
      d3 = d*d2;
      for(k=0; k<3; ++k) {
        double f = -rij[k]/d3;

        forces[i][k] += f;

        forces[j][k] -= f;
      }
      ene += -1.0/d;
    }
  }
}
```



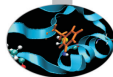
Nbody

Fortran

```
do i = 1, DIM
  do j = i+1, DIM
    rij(:) = pos(:,i) - pos(:,j)
    d2 = 0.d0
    do k = 1, 3
      d2 = d2 + rij(k)**2
    end do
    if (d2 .le. cut2) then
      d = sqrt(d2)
      f(:) = - 1.d0 / d**3 * rij(:)
      do k=1, 3

        forces(k,i) = forces(k,i) + f(k)

        forces(k,j) = forces(k,j) - f(k)
      end do
      ene = ene + (-1.d0/d)
    end if
  end do
end do
```



Nbody

C

```
#pragma omp parallel for private(i, j, k, rij, d, d2, d3) reduction(+:ene)
for(i=0; i<nbodies; ++i)
  for(j=i+1; j<nbodies; ++j) {
    d2 = 0.0;
    for(k=0; k<3; ++k) {
      rij[k] = pos[i][k] - pos[j][k];
      d2 += rij[k]*rij[k];
    }
    if (d2 <= cut2) {
      d = sqrt(d2);
      d3 = d*d2;
      for(k=0; k<3; ++k) {
        double f = -rij[k]/d3;

        forces[i][k] += f;

        forces[j][k] -= f;
      }
      ene += -1.0/d;
    }
  }
}
```




Nbody atomic

C

```

#pragma omp parallel for private(i, j, k, rij, d, d2, d3) reduction(+:ene)
  for(i=0; i<nbodies; ++i)
    for(j=i+1; j<nbodies; ++j) {
      d2 = 0.0;
      for(k=0; k<3; ++k) {
        rij[k] = pos[i][k] - pos[j][k];
        d2 += rij[k]*rij[k];
      }
      if (d2 <= cut2) {
        d = sqrt(d2);
        d3 = d*d2;
        for(k=0; k<3; ++k) {
          double f = -rij[k]/d3;
          #pragma omp atomic
          forces[i][k] += f;
          #pragma omp atomic
          forces[j][k] -= f;
        }
        ene += -1.0/d;
      }
    }
  }

```



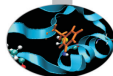
Nbody atomic

C

```

#pragma omp parallel for private(i,j,k,rij,d,d2,d3) reduction(+:ene) \
schedule(guided)
  for(i=0; i<nbodies; ++i)
    for(j=i+1; j<nbodies; ++j) {
      d2 = 0.0;
      for(k=0; k<3; ++k) {
        rij[k] = pos[i][k] - pos[j][k];
        d2 += rij[k]*rij[k];
      }
      if (d2 <= cut2) {
        d = sqrt(d2);
        d3 = d*d2;
        for(k=0; k<3; ++k) {
          double f = -rij[k]/d3;
          #pragma omp atomic
          forces[i][k] += f;
          #pragma omp atomic
          forces[j][k] -= f;
        }
        ene += -1.0/d;
      }
    }
  }

```



Nbody

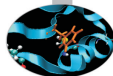
Fortran

```

!$omp parallel do private(i,j,k,rij,d,d2,f) reduction(+:ene)
  do i = 1, DIM
    do j = i+1, DIM
      rij(:) = pos(:,i) - pos(:,j)
      d2 = 0.d0
      do k = 1, 3
        d2 = d2 + rij(k)**2
      end do
      if (d2 .le. cut2) then
        d = sqrt(d2)
        f(:) = - 1.d0 / d**3 * rij(:)
        do k=1, 3

          forces(k,i) = forces(k,i) + f(k)

          forces(k,j) = forces(k,j) - f(k)
        end do
        ene = ene + (-1.d0/d)
      end if
    end do
  end do
!$omp end parallel do
  
```

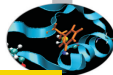


Nbody atomic

Fortran

```

!$omp parallel do private(i,j,k,rij,d,d2,f) reduction(+:ene)
  do i = 1, DIM
    do j = i+1, DIM
      rij(:) = pos(:,i) - pos(:,j)
      d2 = 0.d0
      do k = 1, 3
        d2 = d2 + rij(k)**2
      end do
      if (d2 .le. cut2) then
        d = sqrt(d2)
        f(:) = - 1.d0 / d**3 * rij(:)
        do k=1, 3
          !$omp atomic
          forces(k,i) = forces(k,i) + f(k)
          !$omp atomic
          forces(k,j) = forces(k,j) - f(k)
        end do
        ene = ene + (-1.d0/d)
      end if
    end do
  end do
!$omp end parallel do
  
```



Nbody atomic

Fortran

```

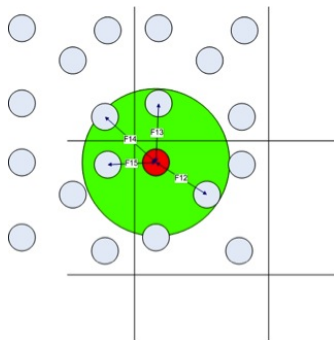
!$omp parallel do private(i,j,k,rij,d,d2,f) reduction(+:ene) &
!$omp schedule(guided)
  do i = 1, DIM
    do j = i+1, DIM
      rij(:) = pos(:,i) - pos(:,j)
      d2 = 0.d0
      do k = 1, 3
        d2 = d2 + rij(k)**2
      end do
      if (d2 .le. cut2) then
        d = sqrt(d2)
        f(:) = - 1.d0 / d**3 * rij(:)
        do k=1, 3
          !$omp atomic
            forces(k,i) = forces(k,i) + f(k)
          !$omp atomic
            forces(k,j) = forces(k,j) - f(k)
        end do
        ene = ene + (-1.d0/d)
      end if
    end do
  end do
!$omp end parallel do
  
```



When the Going Gets Tough, ...

5 Parallelize the serial code **Nbody**. It computes the total energy and the forces of a system of N particles with potential $V = 1/r$ if r is less of a threshold and $V = 0$ otherwise.

- pay attention to the update of **forces**
 - try to update them atomically
 - **try to reduce them**
- try different schedules and test their performance



• to compile use the preprocessing MACRO DIM=55000, for example

```
* gcc -O3 -DDIM=55000 Nbody.c -o nbody -lm
```



Nbody hand reduced in C

C ...

```
int tot_threads;
double ( *gforces ) [3];

#pragma omp parallel private(i, j, k, rij, d, d2, d3)
{
#ifdef _OPENMP
    tot_threads = omp_get_num_threads();
#else
    tot_threads = 1;
#endif
    #pragma omp single
        gforces = calloc(nbodies*tot_threads, \
            sizeof( *gforces ));

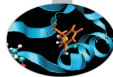
    double ( *pforces ) [3];

#ifdef _OPENMP
        pforces = gforces + nbodies*omp_get_thread_num();
    #else
        pforces = gforces;
    #endif
}
```

C

```
#pragma omp for reduction(+:ene) schedule(guided)
for(i=0; i<nbodies; ++i)
    for(j=i+1; j<nbodies; ++j) {
        d2 = 0.0;
        for(k=0; k<3; ++k) {
            rij[k] = pos[i][k] - pos[j][k];
            d2 += rij[k]*rij[k];
        }
        if (d2 <= cut2) {
            d = sqrt(d2);
            d3 = d*d2;
            for(k=0; k<3; ++k) {
                double f = -rij[k]/d3;
                pforces[i][k] += f;
                pforces[j][k] -= f;
            }
            ene += -1.0/d;
        }
    }

for(i=0; i<nbodies; ++i)
    for (j=0; j<tot_threads; j++)
        for(k=0; k<3; ++k)
            forces[i][k] += gforces[i+j*nbodies][k];
}
```



Nbody hand reduced in C

```
C ...
int tot_threads;
double ( *gforces ) [3];

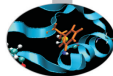
#pragma omp parallel private(i, j, k, rij, d, d2, d3)
{
#ifdef _OPENMP
    tot_threads = omp_get_num_threads();
#else
    tot_threads = 1;
#endif
    #pragma omp single
    gforces = calloc(nbodies*tot_threads, \
        sizeof( *gforces ));

    double ( *pforces ) [3];

#ifdef _OPENMP
    pforces = gforces + nbodies*omp_get_thread_num();
#else
    pforces = gforces;
#endif
}
```

```
C
#pragma omp for reduction(+:ene) schedule(guided)
for(i=0; i<nbodies; ++i)
    for(j=i+1; j<nbodies; ++j) {
        d2 = 0.0;
        for(k=0; k<3; ++k) {
            rij[k] = pos[i][k] - pos[j][k];
            d2 += rij[k]*rij[k];
        }
        if (d2 <= cut2) {
            d = sqrt(d2);
            d3 = d*d2;
            for(k=0; k<3; ++k) {
                double f = -rij[k]/d3;
                pforces[i][k] += f;
                pforces[j][k] -= f;
            }
            ene += -1.0/d;
        }
    }

for(i=0; i<nbodies; ++i)
    for (j=0; j<tot_threads; j++)
        for(k=0; k<3; ++k)
            forces[i][k] += gforces[i+j*nbodies][k];
}
```

Nbody hand reduced in C

```
C ...
int tot_threads;
double ( *gforces ) [3];

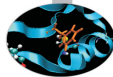
#pragma omp parallel private(i, j, k, rij, d, d2, d3)
{
#ifdef _OPENMP
    tot_threads = omp_get_num_threads();
#else
    tot_threads = 1;
#endif
    #pragma omp single
        gforces = calloc(nbodies*tot_threads, \
            sizeof( *gforces ));

        double ( *pforces ) [3];

#ifdef _OPENMP
    pforces = gforces + nbodies*omp_get_thread_num();
#else
    pforces = gforces;
#endif
}
```

```
C
#pragma omp for reduction(+:ene) schedule(guided)
for(i=0; i<nbodies; ++i)
    for(j=i+1; j<nbodies; ++j) {
        d2 = 0.0;
        for(k=0; k<3; ++k) {
            rij[k] = pos[i][k] - pos[j][k];
            d2 += rij[k]*rij[k];
        }
        if (d2 <= cut2) {
            d = sqrt(d2);
            d3 = d*d2;
            for(k=0; k<3; ++k) {
                double f = -rij[k]/d3;
                pforces[i][k] += f;
                pforces[j][k] -= f;
            }
            ene += -1.0/d;
        }
    }

for(i=0; i<nbodies; ++i)
    for (j=0; j<tot_threads; j++)
        for(k=0; k<3; ++k)
            forces[i][k] += gforces[i+j*nbodies][k];
}
```



Nbody hand reduced in C

```
C ...
int tot_threads;
double ( *gforces ) [3];

#pragma omp parallel private(i, j, k, rij, d, d2, d3)
{
#ifdef _OPENMP
    tot_threads = omp_get_num_threads();
#else
    tot_threads = 1;
#endif
    #pragma omp single
        gforces = calloc(nbodies*tot_threads, \
            sizeof( *gforces ));

    double ( *pforces ) [3];

#ifdef _OPENMP
    pforces = gforces + nbodies*omp_get_thread_num();
#else
    pforces = gforces;
#endif
#endif
```

```
C
#pragma omp for reduction(+:ene) schedule(guided)
for(i=0; i<nbodies; ++i)
    for(j=i+1; j<nbodies; ++j) {
        d2 = 0.0;
        for(k=0; k<3; ++k) {
            rij[k] = pos[i][k] - pos[j][k];
            d2 += rij[k]*rij[k];
        }
        if (d2 <= cut2) {
            d = sqrt(d2);
            d3 = d*d2;
            for(k=0; k<3; ++k) {
                double f = -rij[k]/d3;
                pforces[i][k] += f;
                pforces[j][k] -= f;
            }
            ene += -1.0/d;
        }
    }
#pragma omp for
for(i=0; i<nbodies; ++i)
    for (j=0; j<tot_threads; j++)
        for(k=0; k<3; ++k)
            forces[i][k] += gforces[i+j*nbodies][k];
}
```



Nbody reduction in Fortran

Fortran

```

!$omp parallel do private(i,j,k,rij,d,d2,f) &
!$omp reduction(+:ene,forces) &
!$omp schedule(guided)
  do i = 1, DIM
    do j = i+1, DIM
      rij(:) = pos(:,i) - pos(:,j)
      d2 = 0.d0
      do k = 1, 3
        d2 = d2 + rij(k)**2
      end do
      if (d2 .le. cut2) then
        d = sqrt(d2)
        f(:) = - 1.d0 / d**3 * rij(:)
        forces(:,i) = forces(:,i) + f(:)
        forces(:,j) = forces(:,j) - f(:)
        ene = ene + (-1.d0/d)
      end if
    end do
  end do
!$omp end parallel do
  
```