Суперкомпьютеры и параллельная обработка данных

Бахтин Владимир Александрович
к.ф.-м.н., ведущий научный сотрудник
Института прикладной математики им М.В.Келдыша РАН
кафедра системного программирования
факультет вычислительной математики и кибернетики
Московского университета им. М.В. Ломоносова

Содержание

Новые возможности OpenMP

- Векторизация кода
- Обработка исключительных ситуаций / cancellation constructs
- Поддержка ускорителей/сопроцессоров

Использование векторизации

```
void add_float (float *a, float *b, float *c, float *d, float *e, int n)
{
    for (int i=0; i<n; i++)
      a[i] = a[i] + b[i] + c[i] + d[i] + e[i];
}
```

Использование векторизации

```
void add_float (float *restrict a, float *restrict b, float *restrict c,
float *restrict d, float *restrict e, int n) // C99
{
    for (int i=0; i<n; i++)
      a[i] = a[i] + b[i] + c[i] + d[i] + e[i];
}
```

Использование векторизации. Спецификация simd

#pragma omp simd *[clause[[,] clause]..]*
**   *for-loops***

#pragma omp for simd *[clause[[,] clause]..]*
**   *for-loops***

где клауза одна из:

- **safelen (length)**
- **linear (list[:linear-step])**
- **aligned (list[:alignment])**
- **private (list)**
- **lastprivate (list)**
- **reduction (reduction-identifier: list)**
- **collapse (n)**

Использование векторизации

```
void add_float (float *a, float *b, float *c, float *d, float *e, int n)
{
  #pragma omp simd
  for (int i=0; i<n; i++)
    a[i] = a[i] + b[i] + c[i] + d[i] + e[i];
}


void add_float (float *restrict a, float *restrict b, float *restrict c,
float *restrict d, float *restrict e, int n) // C99
{
   for (int i=0; i<n; i++)
    a[i] = a[i] + b[i] + c[i] + d[i] + e[i];
}
```

Использование векторизации. Спецификация declare simd

#pragma omp declare simd ***[clause[[,] clause]..]***
function definition or declaration

где клауза одна из:

- **simdlen (length)**
  the largest size for a vector that the compiler is free to assume
- **linear (argument-list[:constant-linear-step])**
  in serial execution parameters are incremented by steps (induction variables with constant stride)
- **aligned (argument-list[:alignment])**
  all arguments in the argument-list are aligned on a known boundary not less than the specified alignment
- **uniform (argument-list)**
  shared, scalar parameters are broadcasted to all iterations
- **inbranch**
- **notinbranch**

Использование векторизации

```
#pragma omp declare simd notinbranch
float min(float a, float b) {
  return a < b ? a : b;
}

#pragma omp declare simd inbranch
float distance (float x, float y) {
  return (x - y) * (x - y);
}

#pragma omp parallel for simd
for (i=0; i<N; i++)
  d[i] = min (distance (a[i], b[i]), c[i]);
```

Cancellation Constructs

Директива

#pragma omp cancel *clause[[,] clause]*
где clause одна из:

- ❑ **parallel**
- ❑ **sections**
- ❑ **for**
- ❑ **taskgroup**
- ❑ **if (***scalar-expression***)**

Директива

#pragma omp cancellation point *clause[[,] clause]*
где clause одна из:

- ❑ **parallel**
- ❑ **sections**
- ❑ **for**
- ❑ **taskgroup**

Новая функция системы поддержки:

- ❑ **omp_get_cancellation**

Новая переменная окружения:

- ❑ **OMP_CANCELLATION**

Обработка исключительных ситуаций

```
void example() {
    std::exception *ex = NULL;
    #pragma omp parallel shared(ex)
    {
        #pragma omp for schedule(runtime)
        for (int i = 0; i < N; i++) {
            try {
                causes_an_exception();
            } catch (std::exception *e) {
                #pragma omp atomic write
                   ex = e; // still must remember exception for later handling
               #pragma omp cancel for // cancel worksharing construct
            }
        }
        if (ex) { // if an exception has been raised, cancel parallel region
           #pragma omp cancel parallel
        }
   }
   if (ex) {  // handle exception stored in ex
   }
}
```

Поиск в дереве (часть 1)

```
typedef struct binary_tree_s {
  int value;
  struct binary_tree_s *left, *right;
} binary_tree_t;

binary_tree_t *search_tree_parallel (binary_tree_t *tree, int value) {
   binary_tree_t *found = NULL;
#pragma omp parallel shared(found, tree, value)
   {
#pragma omp taskgroup
      {
#pragma omp master
         {
            found = search_tree(tree, value, 0);
         }
      }
   }
   return found;
}
```

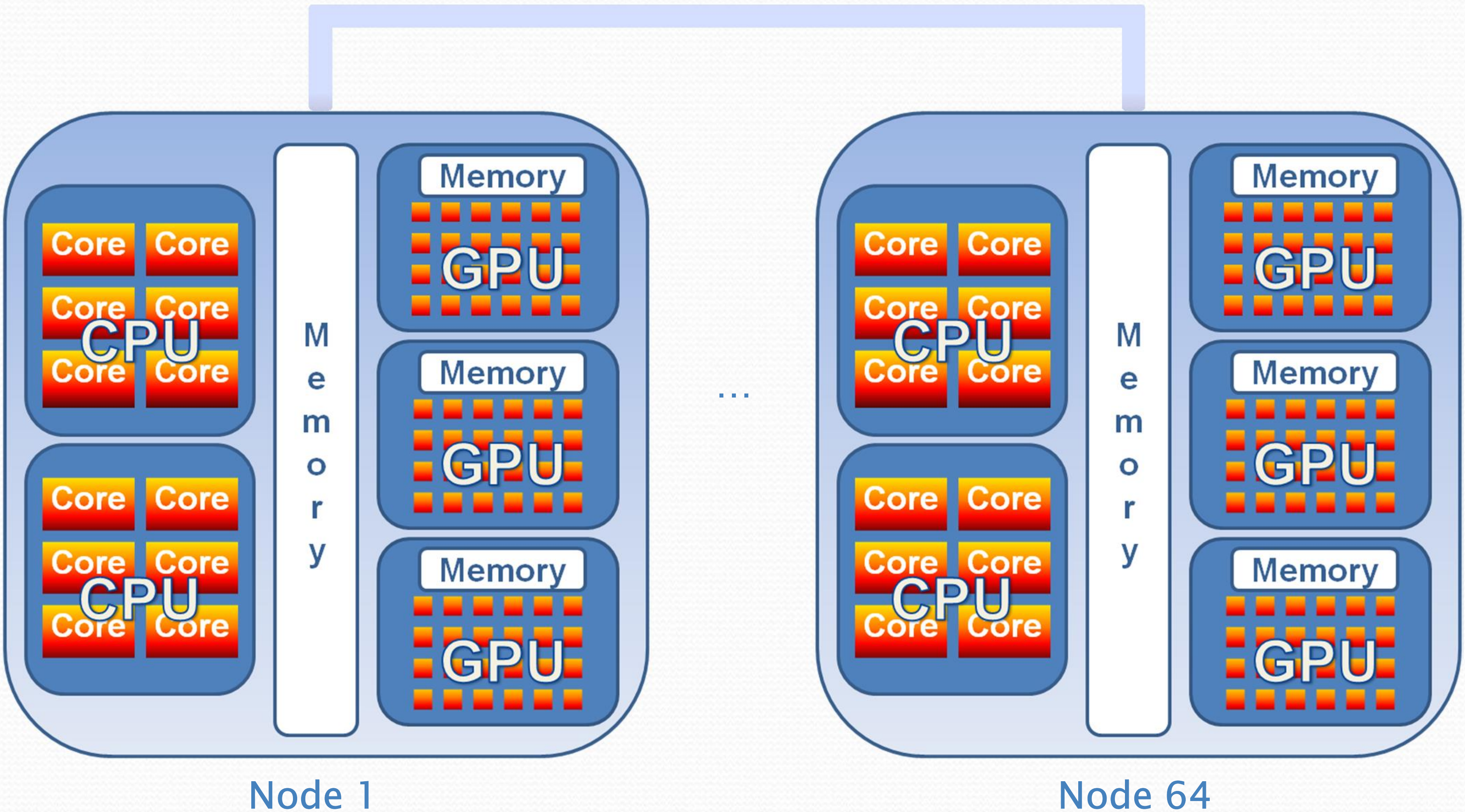
Поиск в дереве (часть 2)

```
binary_tree_t *search_tree(binary_tree_t *tree, int value, int level) {
    binary_tree_t *found = NULL;
    if (tree) {
        if (tree->value == value) {
            found = tree;
        } else {
            #pragma omp task shared(found) if(level < 10)
            {
                binary_tree_t *found_left = NULL;
                found_left = search_tree(tree->left, value, level + 1);
                if (found_left) {
                    #pragma omp atomic write
                      found = found_left;
                    #pragma omp cancel taskgroup
                }
            }
```

Поиск в дереве (часть 3)

```
            #pragma omp task shared(found) if(level < 10)
            {
               binary_tree_t *found_right = NULL;
               found_right = search_tree(tree->right, value, level + 1);
               if (found_right) {
                  #pragma omp atomic write
                     found = found_right;
                  #pragma omp cancel taskgroup
               }
            }
           #pragma omp taskwait
        }
     }
     return found;
}
```

Расширение OpenMP для использования ускорителей



Алгоритм Якоби на языке Fortran

```
PROGRAM    JACOB_SEQ
PARAMETER    (L=4096,  ITMAX=100)
REAL     A(L,L), B(L,L)
PRINT *,  '**********  TEST_JACOBI   **********'
DO IT  =  1,  ITMAX
      DO  J  =  2, L-1
              DO  I  =  2, L-1
                     A(I, J)  =  B(I, J)
              ENDDO
      ENDDO
      DO  J = 2,  L-1
             DO  I = 2,  L-1
                    B(I, J) =  (A(I-1, J) + A(I, J-1) +  A(I+1, J) +
*                                  A(I, J+1)) / 4
             ENDDO
       ENDDO
 ENDDO
 END
```

Алгоритм Якоби на языке Fortran Cuda

```
PROGRAM JACOB_CUDA
    use cudafor
    use jac_cuda
    PARAMETER (L=4096,  ITMAX=100)
    parameter (block_dim = 16)
    real, device, dimension(l, l) :: a, b
    type(dim3) :: grid, block
    PRINT *, '*****   TEST_JACOBI   *******'
    grid = dim3(l / block_dim, l / block_dim, 1)
    block = dim3(block_dim, block_dim, 1)
    DO IT = 1, ITMAX
       call arr_copy<<<grid, block>>>(a, b, l)
       call arr_renew<<<grid, block>>>(a, b, l)
    ENDDO
END
```

Алгоритм Якоби на языке Fortran Cuda

```
module jac_cuda
      contains
      attributes(global) subroutine arr_copy(a, b, k)
        real, device, dimension(k, k) :: a, b
        integer, value :: k
        integer i, j
        i = (blockIdx%x - 1) * blockDim%x + threadIdx%x
        j = (blockIdx%y - 1) * blockDim%y + threadIdx%y
        if (i.ne.1 .and. i.ne.k .and. j.ne.1 .and. j.ne.k) A(I, J) = B(I, J)
      end subroutine arr_copy
      attributes(global) subroutine arr_renew(a, b, k)
        real, device, dimension(k, k) :: a, b
        integer, value :: k
        integer i, j
        i = (blockIdx%x - 1) * blockDim%x + threadIdx%x
        j = (blockIdx%y - 1) * blockDim%y + threadIdx%y
       if (i.ne.1 .and. i.ne.k .and. j.ne.1 .and. j.ne.k)  B(I,J) =(A( I-1,J)+A(I,J-1)+A(I+1,J)+
A(I,J+1))/4
      end subroutine arr_renew
end module jac_cuda
```

Алгоритм Якоби в модели HMPP

```
!$HMPP jacoby codelet, target = CUDA
        SUBROUTINE JACOBY(A,B,L)
        IMPLICIT NONE
        INTEGER, INTENT(IN) :: L
        REAL, INTENT(IN) :: A(L,L)
        REAL, INTENT(INOUT) :: B(L,L)
        INTEGER I,J
        DO  J  =  2, L-1
              DO  I  =  2, L-1
                    A(I,J)  =  B(I,J)
              ENDDO
        ENDDO
          DO  J = 2,  L-1
               DO  I = 2,  L-1
                    B(I,J) =  (A(I-1,J ) + A(I,J-1 ) +
    *                      A(I+1,J ) + A(I,J+1 )) / 4
             ENDDO
          ENDDO
        END SUBROUTINE JACOBY
```

```
      PROGRAM JACOBY_HMPP
      PARAMETER    (L=4096,  ITMAX=100)
      REAL     A(L,L), B(L,L)
      PRINT *,   '**********TEST_JACOBI**********'
      DO IT  =  1,  ITMAX
!$HMPP    jacoby callsite
        CALL JACOBY(A,B,L)
      ENDDO
      PRINT *, B
      END
```

Алгоритм Якоби в модели HMPP

```
          PROGRAM    JACOBY_HMPP
           PARAMETER    (L=4096,  ITMAX=100)
           REAL     A(L,L), B(L,L)
!$hmpp jac allocate, args[A;B].size={L,L}
!$hmpp jac advancedload, args[B]
            PRINT *,  '**********  TEST_JACOBI   **********'
            DO IT  =  1,  ITMAX
!$hmpp jac region, args[A;B].noupdate=true
                DO  J  =  2, L-1
                    DO  I  =  2, L-1
                        A(I, J)  =  B(I, J)
                    ENDDO
                ENDDO
                 DO  J = 2,  L-1
                    DO  I = 2,  L-1
                        B(I, J)=(A(I-1,J)+A(I,J-1)+A(I+1,J) +
            *                A(I, J+1)) / 4
                     ENDDO
                 ENDDO
 !$hmpp jac endregion
            ENDDO
 !$hmpp jac delegatedstore, args[B]
 !$hmpp jac release
            PRINT *,B
            END
```

Алгоритм Якоби в модели PGI APM

```
       PROGRAM JACOBY_PGI_APM
       PARAMETER    (L=4096,  ITMAX=100)
       REAL    A(L,L), B(L,L)
       PRINT *,  '**********  TEST_JACOBI   **********'
!$acc data region copyin(B), copyout(B), local(A)
       DO IT  =  1,  ITMAX
!$acc      region
              DO  J  =  2, L-1
                     DO  I  =  2, L-1
                            A(I,J)  =  B(I,J)
                     ENDDO
              ENDDO
              DO  J = 2,  L-1
                     DO  I = 2,  L-1
                            B(I,J) =  (A(I-1,J ) + A(I,J-1 ) + A(I+1,J ) + A(I,J+1 )) / 4
                     ENDDO
              ENDDO
!$acc      end  region
       ENDDO
!$acc end data region
       PRINT *, B
       END
```

Cray Compiling Environment 7.4.0

```
!$omp acc_region
!$omp acc_loop
          DO j = 1,M
            DO i = 2,N
               c(i,j) = a(i,j) + b(i,j)
            ENDDO
          ENDDO
!$omp end acc_loop
!$omp end acc_region
```

acc_region:

acc_copy, acc_copyin, acc_copyout, acc_shared, private, firstprivate, default(<any of above>|none), present, if(scalar-logical-expression), device(integer-expression), num_pes(depth:num [, depth:num]), async(handle)

acc_loop:

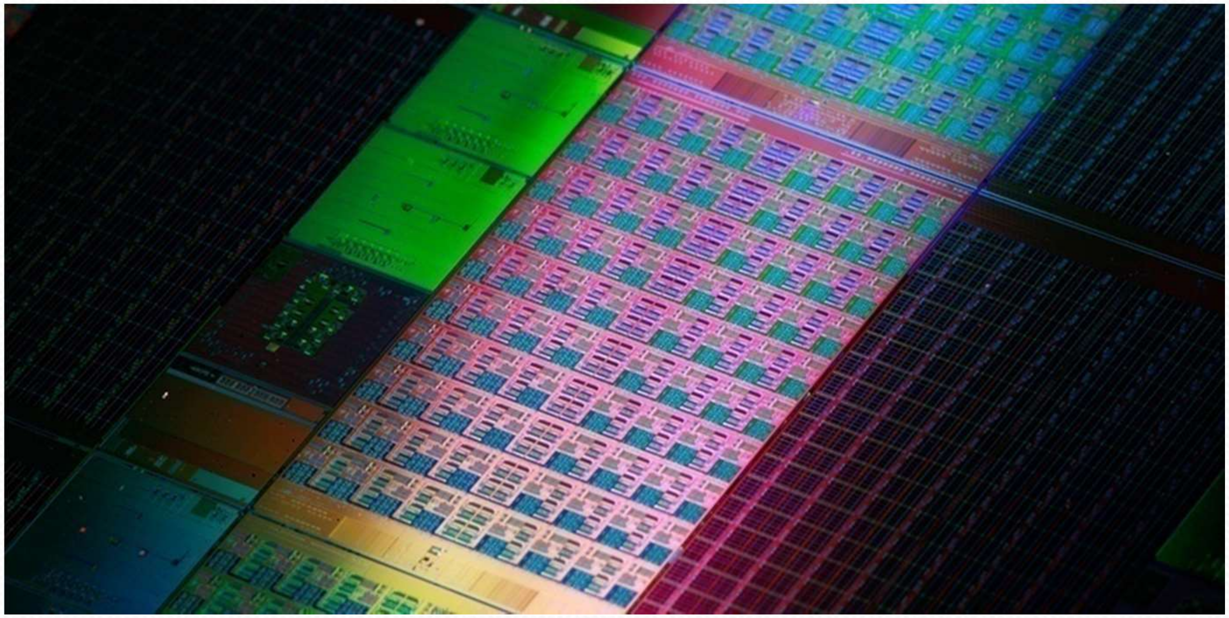
reduction(operator:list), collapse(n), schedule, cache(obj[:depth], hetero…

OpenACC

```
#pragma acc data copy(A), create(Anew)
while (iter<iter_max) {
  #pragma acc kernels loop
  for (int j = 1; j < n-1; j++) {
     for (int I = 1; I < m-1; i++) {
        Anew[j][i] = 0.25* (A[j][i+1] + A[j][i-1] +A[j-1][i] + A[j+1][i]);
     }
   }
  #pragma acc kernels loop
  for (int j = 1; j < n-1; j++) {
     for (int I = 1; i< m-1;i++ ) {
       A[j][i] = Anew[j][i];
     }
  }
  iter++;
}
```

Intel Many Integrated Core (MIC)

```
!dir$ offload target(mic)
!$omp parallel do
          do i=1,10
              A(i) = B(i) * C(i)
          enddo
!$omp end parallel
```



OpenMP accelerator model

Новые директивы
- target
- target data
- target update
- teams
- distribute

Новые функции системы поддержки
- omp_get_num_devices
- omp_set_default_device
- omp_get_default_device
- omp_is_initial_device
- omp_get_num_teams
- omp_get_team_num

Новая переменная окружения
- OMP_DEFAULT_DEVICE

OpenMP accelerator model. Директива target

#pragma omp target *[clause[[,] clause]]*
structured-block

где clause одна из:
- **device(***integer-expression***)**
- **map** *([map-type]:list)*

map-type:
  - **alloc**
  - **to**
  - **from**
  - **tofrom (по умолчанию)**
- **if (***scalar-expression***)**

```
sum=0;
#pragma omp target device(acc0) map(A,B)
#pragma omp parallel for reduction(+: sum)
  for (i=0;i<N;i++)
      sum += A[i]*B[i];
```

OpenMP accelerator model

#pragma omp target data *[clause[[,] clause]]*

structured-block

где clause одна из:

❑**device(***integer-expression***)**
❑**map** *([map-type]:list)*
map-type:

- **alloc**
- **to**
- **from**
- **tofrom**

❑**if (***scalar-expression***)**

#pragma omp target update*[clause[[,] clause]]*

где clause одна из:

❑**to** *(list)*
❑**from** *(list)*
❑**device(***integer-expression***)**
❑**if (***scalar-expression***)**

OpenMP accelerator model. Директива target data

```
#pragma omp target data device(acc0) map(alloc: tmp[0:N]) \
        map(to: input[:N]) map(from: output)
{
  #pragma omp target device(acc0)
  #pragma omp parallel for
    for (int i=0; i<N; i++)
        tmp[i] = some_device_computation (input[i]);

  input[0] = some_host_computation ();
  #pragma omp target update to (input[0]) device(acc0)

  #pragma omp target device(acc0)
  #pragma omp parallel for reduction(+: output)
     for (int i=0; i<N; i++) output += final_device_computation (tmp[i], input[i])
}
```

OpenMP accelerator model. Директива declare target

```
#pragma omp declare target
   function-defenition-or-declaration

#pragma omp declare target
   float Q[N][N];
   #pragma omp declare simd uniform(i) linear(j) notinbranch
   float func(const int i, const int j)
   {
      return Q[i][j] * Q[j][i];
   }
#pragma omp end declare target

…
#pragma omp target
#pragma omp parallel for reduction(+: sum)
  for (int i=0; i < N; i++) {
    for (int j=0; j < N; j++) {
        sum += func (i,j);
    }
  }

…
```

OpenMP accelerator model. Директива teams

#pragma omp teams *[clause[[,]clause] ,...]*
structured-block

где clause одна из:

- **num_teams** *(integer-expression)*
- **thread_limit** *(integer-expression)*
- **private** *(list)*
- **firstprivate** *(list)*
- **shared** *(list)*
- **default (shared | none)**
- **reduction** *(reduction-identifier: list)*

Использование директивы teams

```
float dotprod(float B[], float C[], int N)
{
  float sum0 = 0.0, sum1 = 0.0;
  #pragma omp target map(to: B[:N], C[:N])
  #pragma omp teams num_teams(2)
  {
    if (omp_get_team_num() == 0)
    {
      #pragma omp parallel for reduction(+:sum0)
      for (int i=0; i<N/2; i++)
        sum0 += B[i] * C[i];
    } else if (omp_get_team_num() == 1) {
      #pragma omp parallel for reduction(+:sum1)
      for (int i=N/2; i<N; i++)
        sum1 += B[i] * C[i];
    }
  }
  return sum0 + sum1;
}
```

OpenMP accelerator model. Директива distribute

#pragma omp distribute *[clause[[,]clause] ,...]*
for-loops

где clause одна из:

- **private** *(list)*
- **firstprivate** *(list)*
- **collapse** *(n)*
- **dist_schedule** *(kind[,: chunk_size]) // kind=static*

Может использоваться внутри конструкции **teams**.

OpenMP accelerator model. Директива distribute

```
float dotprod(float B[], float C[], int N)
{
  float sum = 0;
  int i;
  #pragma omp target teams map(to: B[0:N], C[0:N])
  #pragma omp distribute parallel for reduction(+:sum)
  for (i=0; i<N; i++)
    sum += B[i] * C[i];
  return sum;
}
```

OpenMP accelerator model. Директивы teams&&distribute

```
#pragma omp declare target
extern void func(int, int, int);

#pragma omp target device(0)
#pragma omp teams num_teams(60) num_threads (4)
// 60 physical cores, 4 threads in each team
{
  #pragma omp distribute // this loop is distributed across teams
  for (int i = 0; i < 2048; i++) {
    #pragma omp parallel for // loop is executed in parallel by 4 threads of team
    for (int j = 0; j < 512; j++) {
      #pragma omp simd  // create SIMD vectors for the machine
      for (int k=0; k<32; k++) {
         func (i,j,k);
      }
    }
  }
}
```

OpenMP accelerator model. Умножение векторов

```
extern void func_on_host();
extern void output_on_host(float *,int);
#pragma omp declare target
extern void init_on_device(float *,float *,int);

void vec_mult(float *p, int N, int dev)
{
  float *v1, *v2; int i;
  #pragma omp task shared(v1, v2) depend(out: v1, v2)
  #pragma omp target device(dev) map(v1, v2)
  {
     v1=malloc(N*sizeof(float)); v2=malloc(N*sizeof(float)); init_on_device(v1,v2,N);
  }
  func_on_host (); // execute other work asychronously
  #pragma omp task shared(v1, v2, p) depend(in: v1, v2)
  #pragma omp target device(dev) map(to: v1, v2) map(from: p[0:N])
  {
     #pragma omp parallel for
        for (i=0; i<N; i++) p[i] = v1[i] * v2[i];
     free(v1); free(v2);
  }
  #pragma omp taskwait
  output_on_host(p, N);
}
```