University of Nizhni Novgorod
Faculty of Computational Mathematics & Cybernetics

Introduction to Parallel Programming

Section 12.

Parallel Methods for Partial Differential Equations

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Contents…

Contents

Introduction

- *Partial Differential Equations* (*PDE*) are widely used for developing models in various scientific and technical fields
- Analysis of mathematical models based on differential equations is provided by the numerical methods
- The performed computation is greatly time-consuming

Numerical solving of partial differential equations is a subject of intensive research

Problem Statement

Lets consider the *numerical solving of the Dirichlet problem for the Poisson equation* as **the case study for PDE Calculations**. This problem can be formulated as follows:

$$\begin{cases} \dfrac{\delta^2 u}{\delta x^2} + \dfrac{\delta^2 u}{\delta y^2} = f(x,y), & (x,y) \in D, \\ u(x,y) = g(x,y), & (x,y) \in D^0, \end{cases}$$

$$D = \{(x,y) \in D : 0 \le x, y \le 1\}$$

Methods for Solving the Partial Differential Equations…

- **Method of Finite Differences:**
  - The solution domain is represented as a discrete set (*grid*) of points (*nodes*),
  - The solution sequence uniformly converges to the Dirichlet problem solution, while the solution error is of h^2 order

$$\begin{cases} D_h = \{(x_i, y_j) : x_i = ih,\ y_i = jh,\ 0 \le i, j \le N+1, \\ \qquad h = 1/(N+1), \end{cases}$$

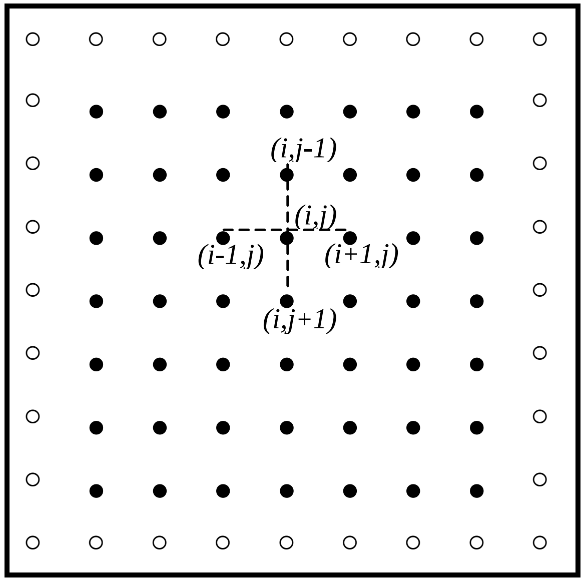
$$\frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{ij}}{h^2} = f_{ij}$$

$$u_{ij} = 0.25\,(u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - h^2 f_{ij})$$

Methods for Solving the Partial Differential Equations…

The Gauss-Seidel method…

$$u_{ij}^{k} = 0.25\,(u_{i-1,j}^{k} + u_{i+1,j}^{k-1} + u_{i,j-1}^{k} + u_{i,j+1}^{k-1} - h^{2} f_{ij})$$



Calculation complexity

T = kmN²

where

- **N** - number of nodes for each dimension,
- **m** - number of operations for one node,
- **k** - number of iterations

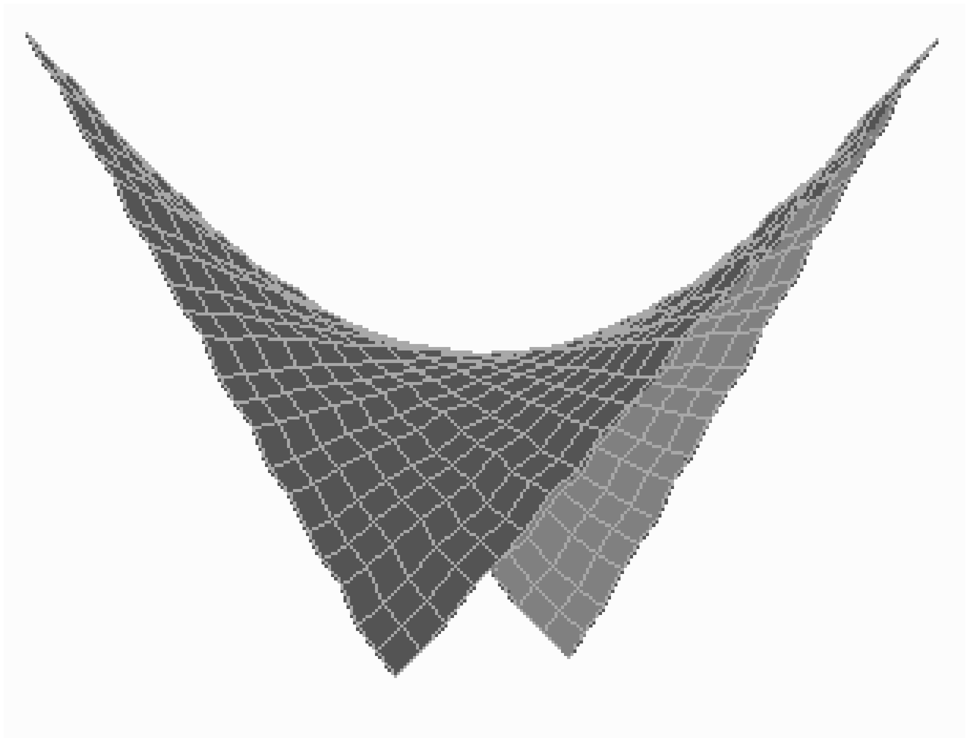
Algorithm 1: *The Sequential Gauss-Seidel Algorithm*

```
// Algorithm 12.1
do {
  dmax = 0; // maximum deviation of values u
  for ( i=1; i<N+1; i++ )
    for ( j=1; j<N+1; j++ ) {
      temp = u[i][j];
      u[i][j] = 0.25*(u[i-1][j]+u[i+1][j]+
                u[i][j-1]+u[i][j+1]–h*h*f[i][j]);
      dm = fabs(temp-u[i][j]);
      if ( dmax < dm ) dmax = dm;
    }
} while ( dmax > eps );
```

Code

A Computational Example

$$\begin{cases} f(x,y)=0, & (x,y)\in D, \\ 100-200x, & y=0, \\ 100-200y, & x=0, \\ -100+200x, & y=1, \\ -100+200y, & x=1, \end{cases}$$



N = 100
ε = 0.1
k = 210

Parallel Computations for Shared Memory Systems…

- The possible way for obtaining software for parallel computations – rewriting the existing sequential programs
- Rewriting can be implemented either automatically by a complier or directly by a programmer
- The second approach prevails as the possibilities of automatic program analysis for generating parallel versions of programs are rather restricted
- The application of new algorithmic languages oriented at parallel programming leads to the necessity for a considerable reprogramming of the existing software

Parallel Computations for Shared Memory Systems…

- The possible problem solution is the application of some means "outside of programming language". For instance, they may be directives or comments which are processed by a special preprocessor before the program is compiled
- Directives can be used to point out different ways to parallelize a program, while ***the original program text remains the same***
- The preprocessor replaces the parallelism directives by some additional program code (as a rule in the form of addressing the procedures of a parallel library)
- If there’s no preprocessor, the compiler would ignore directives and construct the ***original sequential program code***

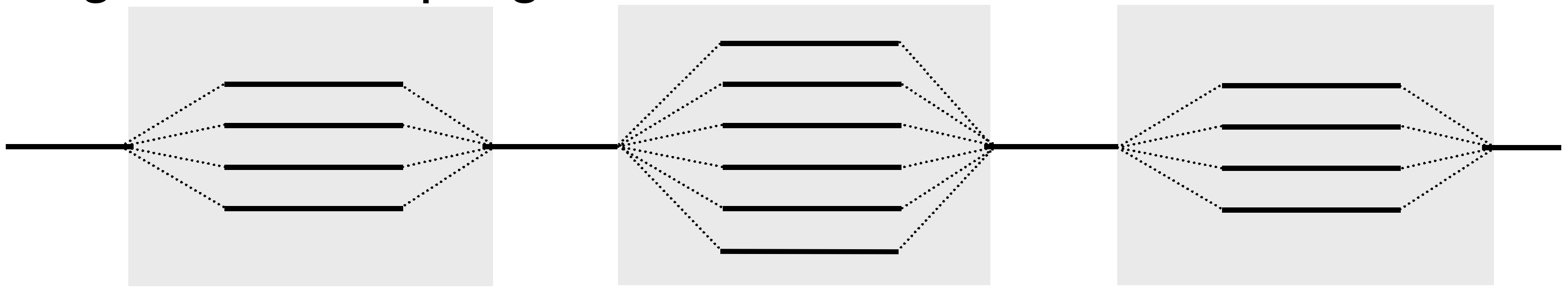
Parallel Computations for Shared Memory Systems

The unity of the program code for sequential and parallel calculations reduces the difficulties in parallel programs' development and maintenance

Conversion of sequential programs to parallel ones by means of directives' application allows to implement the stage-by-stage technology of parallel software development that is greatly valued in programming

OpenMP Technology

- To specify program fragments that can be executed in parallel, the programmer adds directives (C/C++) or comments (Fortran) into the program
- These directives (or comments) allow to determine *the parallel regions* of the program



As a result of this approach the program can be represented as a sequence of interleaved serial (one-thread) and parallel (multi-thread) parts of the code

- Such type of computing is usually referred as *the fork-join* (or *pulsatile*) *parallelism*

Algorithm 1.2: *The first variant of the Gauss-Seidel parallel algorithm*

```
// Algorithm 12.2
omp_lock_t dmax_lock;
omp_init_lock (dmax_lock);
do {
  dmax = 0; // maximum deviation of values u
#pragma omp parallel for shared(u,n,dmax) private(i,temp,d)
  for ( i=1; i<N+1; i++ ) {
#pragma omp parallel for shared(u,n,dmax) private(j,temp,d)
    for ( j=1; j<N+1; j++ ) {
      temp = u[i][j];
      u[i][j] = 0.25*(u[i-1][j]+u[i+1][j]+
                u[i][j-1]+u[i][j+1]–h*h*f[i][j]);
      d = fabs(temp-u[i][j])
      omp_set_lock(dmax_lock);
        if ( dmax < d ) dmax = d;
      omp_unset_lock(dmax_lock);
    } // the end of inner parallel region
  } // the end of outer parallel region
} while ( dmax > eps );
```

Code

The Results of Computational Experiments

Grid size	Gauss-Seidel sequential method (algorithm 12.1)		Parallel algorithm 12.2		
	k	***T***	***k***	***T***	***S***
100	210	0,06	210	1,97	0,03
200	273	0,34	273	11,22	0,03
300	305	0,88	305	29,09	0,03
400	318	3,78	318	54,20	0,07
500	343	6,00	343	85,84	0,07
600	336	8,81	336	126,38	0,07
700	344	12,11	344	178,30	0,07
800	343	16,41	343	234,70	0,07
900	358	20,61	358	295,03	0,07
1000	351	25,59	351	366,16	0,07
2000	367	106,75	367	1585,84	0,07
3000	370	243,00	370	3598,53	0,07

k – the number of iterations,

T – the execution time,

S – the speedup

Estimation of the Approach

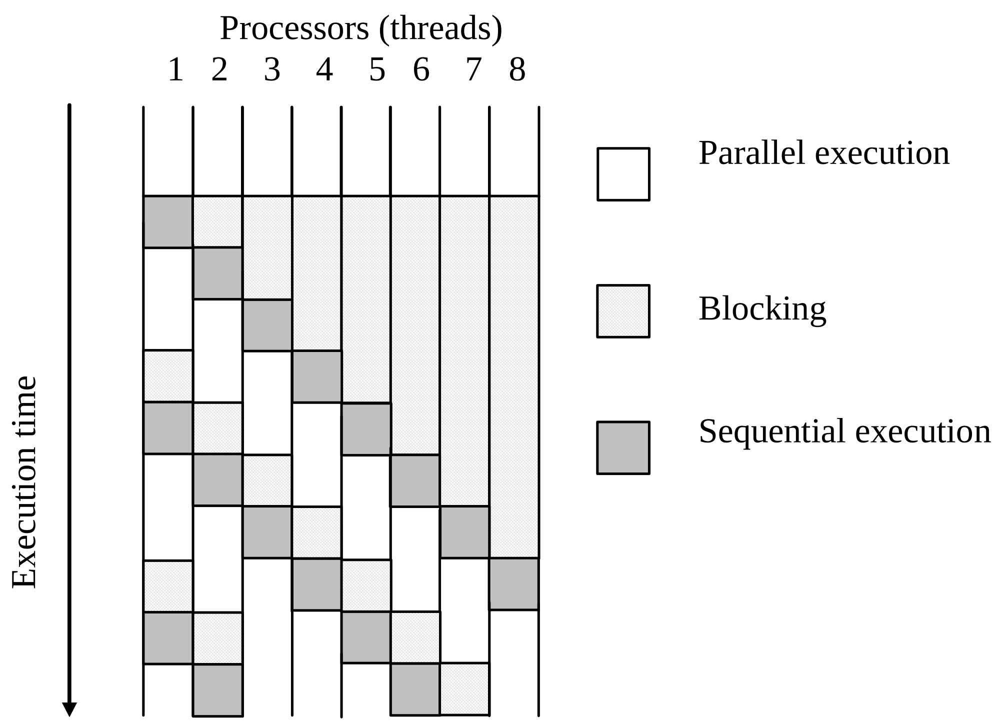
- The developed parallel algorithm provides the solution to the given problem
- It can be used up to N^2 processors for program execution
- There are the excessively high synchronization of the parallel regions of the program
- Low level of processors' load

⇨ ***Low efficiency***

Problem: *Blocking in Mutual Exclusion…*

- Each parallel thread after processing values must check (and probably change) the value d_{max}
- The permission for using the variable has to be obtained by one thread only. The other threads must be blocked. After the shared variable is released the next thread may get control, etc.

Problem: *Blocking in Mutual Exclusion*



As a result a multithread parallel program turns practically into a sequentially executable code

Algorithm 1.3: *The Second Variant of the Gauss-Seidel Parallel Algorithm*

```
// Algorithm 12.3
omp_lock_t dmax_lock;
omp_init_lock(dmax_lock);
do {
  dmax = 0; // maximum deviation of values u
#pragma omp parallel for
shared(u,n,dmax)private(i,temp,d,dm)
  for ( i=1; i<N+1; i++ ) {
    dm = 0;
    for ( j=1; j<N+1; j++ ) {
      temp = u[i][j];
      u[i][j] = 0.25*(u[i-1][j]+u[i+1][j]+
                u[i][j-1]+u[i][j+1]–h*h*f[i][j]);
      d = fabs(temp-u[i][j]);
      if ( dm < d ) dm = d;
    }
    omp_set_lock(dmax_lock);
      if ( dmax < dm ) dmax = dm;
    omp_unset_lock(dmax_lock);
    }
  } // the end of parallel region
} while ( dmax > eps );
```

Code

The Results of Computational Experiments

Grid size	Gauss-Seidel sequential method (algorithm 12.1)		Parallel algorithm 12.2			Parallel algorithm 12.3		
	k	***T***	***k***	***T***	***S***	***k***	***T***	***S***
100	210	0,06	210	1,97	0,03	210	0,03	2,03
200	273	0,34	273	11,22	0,03	273	0,14	2,43
300	305	0,88	305	29,09	0,03	305	0,36	2,43
400	318	3,78	318	54,20	0,07	318	0,64	5,90
500	343	6,00	343	85,84	0,07	343	1,06	5,64
600	336	8,81	336	126,38	0,07	336	1,50	5,88
700	344	12,11	344	178,30	0,07	344	2,42	5,00
800	343	16,41	343	234,70	0,07	343	8,08	2,03
900	358	20,61	358	295,03	0,07	358	11,03	1,87
1000	351	25,59	351	366,16	0,07	351	13,69	1,87
2000	367	106,75	367	1585,84	0,07	367	56,63	1,89
3000	370	243,00	370	3598,53	0,07	370	128,66	1,89

Estimation of the Approach

- ❑ Considerable decrease in the number of shared variable access
- ❑ The maximum possible parallelism decreases to the level of *N*
- ❑ As a result – a considerable decrease in costs of thread synchronization and a decrease of computation serialization effect

⇘ *The best speedup parameters*

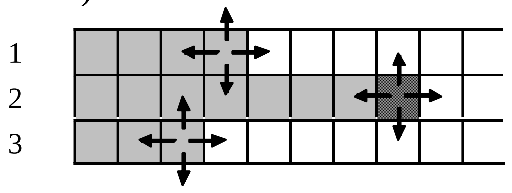
Problem: *Indeterminacy in Parallel Calculations*

- The generated sequence of data processing may vary at several program executions with the same initial data
- The location of threads in the problem domain ***D*** may be different - some threads may pass ahead the others and vice versa
- This tread location structure can vary from execution to execution. The reason of such behavior is *a race condition of threads*

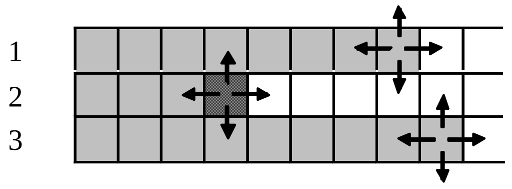
The time dynamics of parallel thread execution should not have an influence on calculations carried out by parallel algorithms and programs

Race Condition of Threads

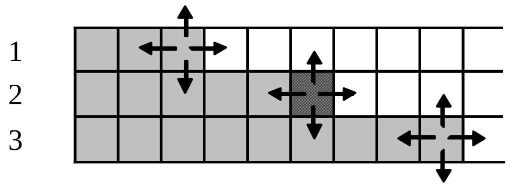
Processors (threads)



Processor 2 passes ahead (the "old" values are used)



Processor 2 lacks behind ("new" values are used)



Processor 2 intermediate ("old" and "new" values are used)

☐ previous iteration values

▨ current iteration

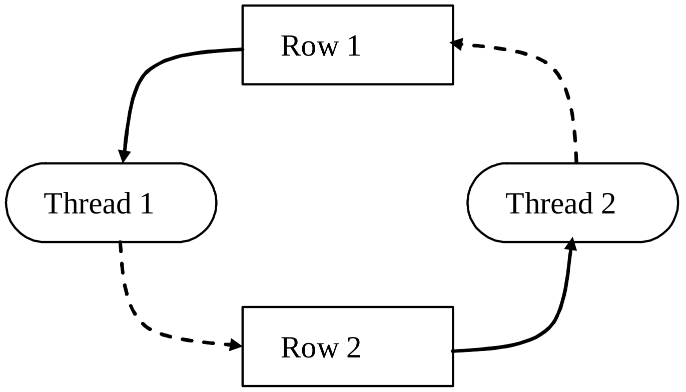
✛ grid nodes, for which the "new" values are executed

A possible solution: ***capture and blocking of the used rows***

Problem: *Deadlocks*

- For the mutual exclusion of access to the grid nodes a set of semaphores **row_lock[N]** may be introduced. It will allow the threads to block the access to their grid rows

```
// the thread is processing the row i
omp_set_lock(row_lock[i]);
omp_set_lock(row_lock[i+1]);
omp_set_lock(row_lock[i-1]);
// processing the grid row i
omp_unset_lock(row_lock[i]);
omp_unset_lock(row_lock[i+1]);
omp_unset_lock(row_lock[i-1]);
```



The threads block first rows 1 and 2 and only then pass over to blocking the rest of the rows – ***deadlock***

Deadlock Avoidance

Approach: the appropriate order in rows’ blocking

```
// the thread is processing the row i
omp_set_lock(row_lock[i+1]);
omp_set_lock(row_lock[i]);
omp_set_lock(row_lock[i-1]);
// < processing the grid row i >
omp_unset_lock(row_lock[i+1]);
omp_unset_lock(row_lock[i]);
omp_unset_lock(row_lock[i-1]);
```

Indeterminacy of calculations is not provided yet

Elimination of Calculation Indeterminacy

- To eliminate calculation indeterminacy the Gauss-Jacobi method can be used, which use separate places to store the results of the previous and the current iterations

Algorithm 1.4: *The Parallel Gauss-Jacobi method…*

```
// Algorithm 12.4
omp_lock_t dmax_lock;
omp_init_lock(dmax_lock);
do {
  dmax = 0; // maximum deviation of values u
#pragma omp parallel for shared(u,n,dmax)\
            private(i,temp,d,dm)
  for ( i=1; i<N+1; i++ ) {
    dm = 0;
    for ( j=1; j<N+1; j++ ) {
      temp = u[i][j];
      un[i][j] = 0.25*(u[i-1][j]+u[i+1][j]+
                 u[i][j-1]+u[i][j+1]–h*h*f[i][j]);
      d = fabs(temp-un[i][j])
      if ( dm < d ) dm = d;
    }
```

to be continued

Algorithm 1.4: *The Parallel Gauss-Jacobi method*

```
    omp_set_lock(dmax_lock);
      if ( dmax < dm ) dmax = dm;
    omp_unset_lock(dmax_lock);
    }
  } // the end of parallel region
  for ( i=1; i<N+1; i++ ) // data update
    for ( j=1; j<N+1; j++ )
      u[i][j] = un[i][j];
} while ( dmax > eps );
```

Code

The results of Computational Experiments

Grid size	Sequential Gauss-Jacobi method (algorithm 12.4)		Parallel Gauss-Jacobi method developed on the analogy of the algorithm 12.3		
	k	*T*	*k*	*T*	*S*
100	5257	1,39	5257	0,73	1,90
200	23067	23,84	23067	11,00	2,17
300	26961	226,23	26961	29,00	7,80
400	34377	562,94	34377	66,25	8,50
500	56941	1330,39	56941	191,95	6,93
600	114342	3815,36	114342	2247,95	1,70
700	64433	2927,88	64433	1699,19	1,72
800	87099	5467,64	87099	2751,73	1,99
900	286188	22759,36	286188	11776,09	1,93
1000	152657	14258,38	152657	7397,60	1,93
2000	337809	134140,64	337809	70312,45	1,91
3000	655210	247726,69	655210	129752,13	1,91

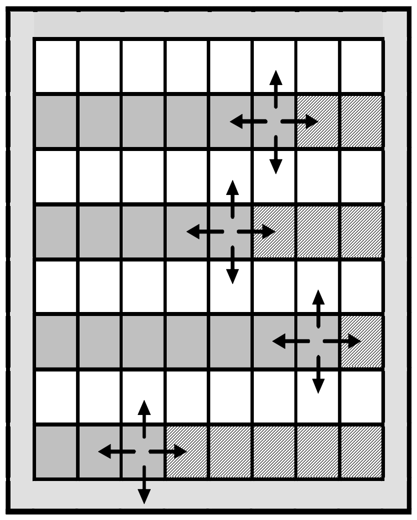
Estimation of the Approach

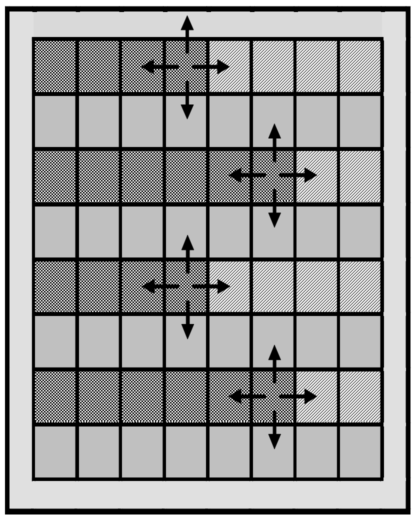
- Uniqueness of the calculations
- Use of the additional memory
- Smaller convergence rate

Another possible approach to eliminate the mutual dependences of parallel threads is to apply *the red/black row alteration scheme*. In this scheme the execution of each iteration is subdivided into two sequential stages:

- At the first stage only the rows with even numbers are processed,
- At the second stage - the rows with odd numbers are used

Red/Black Row Alteration Scheme


Stage 1


Stage 2

⬜	border values	⬜	previous iteration values
▨	values after stage 1 of the current iteration	⬛	values after stage 2 of the current iteration

Estimation of the Approach…

- No additional memory is required
- The algorithm guarantees uniqueness of calculations, which do not coincide with the results obtained by means of sequential algorithm
- Smaller convergence rate

↳ *Potentiality for the increase in the efficiency of calculations*

Estimation of the Approach

The Gauss-Jacobi method	**Red/black row alteration scheme**
Use of the additional memory	Additional memory is not required

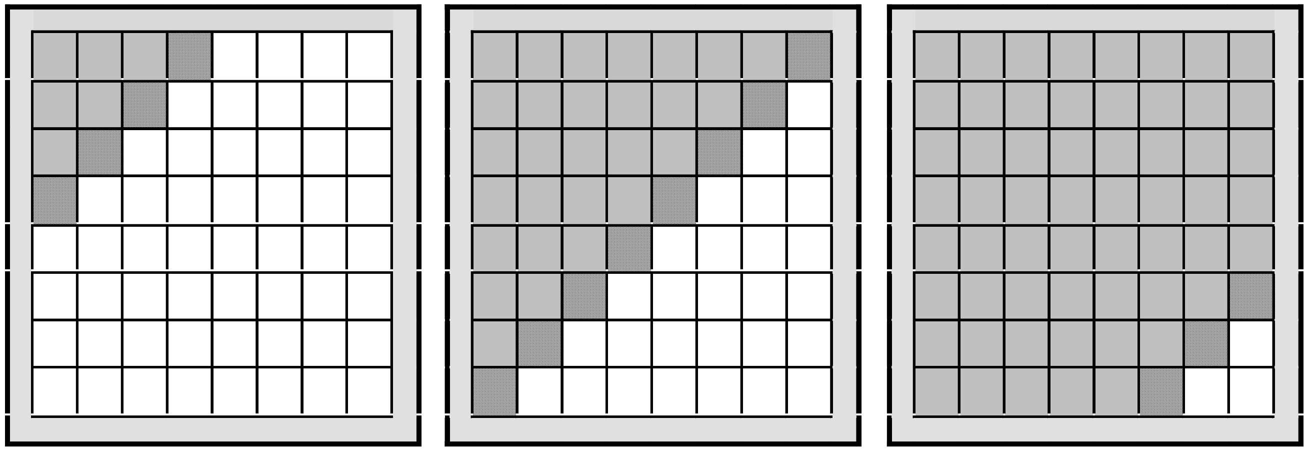
- The algorithm guarantees uniqueness of calculations, though the obtained results may not coincide with the results of the sequential calculations
- Calculation schemes demonstrate the convergence rate, which is worse than the original convergence rate of the Gauss-Seidel method

Parallel Wave Computation Scheme…

- Let us now consider the parallel algorithms with the following characteristics - the performed calculations and the obtained results have to be completely identical to the ones of the original sequential method
- Among such techniques - *the wavefront* or *hyperplane method*
- The wavefront method can be explained as follows – it is evident that to provide calculations identical as at the original sequential method the following should be taken into account:
  - At the first step the node u_{11} may be processed only,
  - Then – at the second step - the node u_{21} and u_{12} may be recalculated, etc.

  As a result at each step the nodes that may be processed form a *bottom-up grid diagonal* with the numbers determined by the step number

Parallel Wave Computation Scheme…



⬜	border values	□	values of the previous iteration
▨	values of the current iteration	■	nodes, at which values can be recalculated

Algorithm 1.5: *Parallel Algorithm Based on Wave Calculation Scheme…*

```
// Algorithm 12.5
omp_lock_t dmax_lock;
omp_init_lock(dmax_lock);
do {
  dmax = 0; // maximum variation of values u
  // growing wave (nx – wave size)
  for ( nx=1; nx<N+1; nx++ ) {
    dm[nx] = 0;
#pragma omp parallel for shared(u,nx,dm) private(i,j,temp,d)
    for ( i=1; i<nx+1; i++ ) {
      j    = nx + 1 – i;
      temp = u[i][j];
      u[i][j] = 0.25*(u[i-1][j]+u[i+1][j]+u[i][j-1]+u[i][j+1]*h*f[i][j]);
      d = fabs(temp-u[i][j])
      if ( dm[i] < d ) dm[i] = d;
    } // the end of parallel region
  }
```

Algorithm 1.5: *Parallel Algorithm Based on Wave Calculation Scheme*

```
// decaying wave
for ( nx=N-1; nx>0; nx-- ) {
#pragma omp parallel for shared(u,nx,dm) private(i,j,temp,d)
    for ( i=N-nx+1; i<N+1; i++ ) {
      j    = 2*N - nx – I + 1;
      temp = u[i][j];
      u[i][j] = 0.25*(u[i-1][j]+u[i+1][j]+u[i][j-1]+u[i][j+1]–h*h*f[i][j]);
      d = fabs(temp-u[i][j])
      if ( dm[i] < d ) dm[i] = d;
    } // the end of parallel region
  }
#pragma omp parallel for shared(n,dm,dmax) private(i)
  for ( i=1; i<nx+1; i++ ) {
    omp_set_lock(dmax_lock);
      if ( dmax < dm[i] ) dmax = dm[i];
    omp_unset_lock(dmax_lock);
  } // the end of parallel region
} while ( dmax > eps );
```

Code

Parallel Wave Computation Scheme

- The final part of calculations for computing the maximum deviation of values *u* is the least efficient due to high additional synchronization cost
- *Chucking* (*fragmentation*) – the technique of increasing sequential computation blocks to reduce the synchronization cost
- The possible variant to implement this approach may be the following:

```
chunk = 200; // sequential part size
#pragma omp parallel for shared(n,dm,dmax)private(i,d)
  for ( i=1; i<nx+1; i+=chunk ) {
    d = 0;
    for ( j=i; j<i+chunk; j++ )
      if ( d < dm[j] ) d = dm[j];
    omp_set_lock(dmax_lock);
      if ( dmax < d ) dmax = d;
    omp_unset_lock(dmax_lock);
} the end of parallel region
```

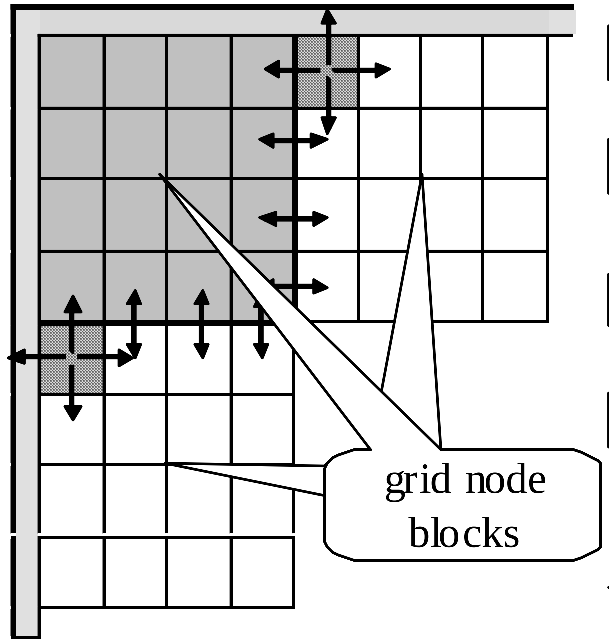
The Results of Computational Experiments

Grid size	Sequential Gauss-Seidel method (algorithm 12.1)		Parallel algorithm 12.5		
	k	***t***	***k***	***t***	***S***
100	210	0,06	210	0,30	0,21
200	273	0,34	273	0,86	0,40
300	305	0,88	305	1,63	0,54
400	318	3,78	318	2,50	1,51
500	343	6,00	343	3,53	1,70
600	336	8,81	336	5,20	1,69
700	344	12,11	344	8,13	1,49
800	343	16,41	343	12,08	1,36
900	358	20,61	358	14,98	1,38
1000	351	25,59	351	18,27	1,40
2000	367	106,75	367	69,08	1,55
3000	370	243,00	370	149,36	1,63

Estimation of the Approach

- Low efficiency of cache use
- In order to increase the computation performance by efficient cache utilization the following conditions need to be provided:
  - The performed calculations use the same data repeatedly (*data processing locality*),
  - The performed calculations provide access to memory elements with sequentially increasing addresses (*sequential access*)
- To meet such requirements the procedure of processing some rectangular *blocks* of the grid should be considered

Block-structured (Checkerboard) Decomposition



⬜	border values
□	previous iteration values
▒	current iteration values
■	nodes which values can be recalculated
⟷	values, which must be transmitted among the block borders

Algorithm 1.6: *Wavefront Method Base on Checkerboard Data Decomposition*

```
//Algorithm 12.6
do {
  // growing wave (wave size is nx+1)
 for ( nx=0; nx<NB; nx++ ) { // NB block number
#pragma omp parallel for shared(nx) private(i,j)
    for ( i=0; i<nx+1; i++ ) {
      j = nx – i;
      // <processing a block with coordinates (i,j)>
    } // the end of parallel region
  }
  // decaying wave
  for ( nx=NB-2; nx>-1; nx-- ) {
#pragma omp parallel for shared(nx) private(i,j)
    for ( i=0; i<nx+1; i++ ) {
      j = 2*(NB-1) - nx – i;
      // <processing a block with coordinates (i,j)>
    } // the end of parallel region
  }
  // <calculation of error estimation >
} while ( dmax > eps );
```

Code

The Results of Calculation Experiments

Grid size	Sequential Gauss-Seidel method (algorithm 12.1)		Parallel algorithm 12.5			Parallel algorithm 12.6		
	K	***T***	***k***	***T***	***S***	***k***	***T***	***S***
100	210	0,06	210	0,30	0,21	210	0,16	0,40
200	273	0,34	273	0,86	0,40	273	0,59	0,58
300	305	0,88	305	1,63	0,54	305	1,53	0,57
400	318	3,78	318	2,50	1,51	318	2,36	1,60
500	343	6,00	343	3,53	1,70	343	4,03	1,49
600	336	8,81	336	5,20	1,69	336	5,34	1,65
700	344	12,11	344	8,13	1,49	344	10,00	1,21
800	343	16,41	343	12,08	1,36	343	12,64	1,30
900	358	20,61	358	14,98	1,38	358	15,59	1,32
1000	351	25,59	351	18,27	1,40	351	19,30	1,33
2000	367	106,75	367	69,08	1,55	367	65,72	1,62
3000	370	243,00	370	149,36	1,63	370	140,89	1,72

Estimation of the Approach

- Block processing is performed on different processors and the blocks are mutually disjoint - as a results there are no additional costs to support for *cache coherency* of different processors
- The situations when processors stay idle are possible

➪ *It is possible to increase the efficiency of calculations*

Processor Load Balancing

- The block size determines *the granularity* of parallel computations
- Choosing the level of granularity it is possible to provide the required efficiency of parallel methods
- To provide the uniform processor loads (*load balancing*) all the computational works can be arranged as *a job queue*
- In the course of computations the processor, which is already unloaded, may ask for a job from the queue

A job queue is the general management scheme of load balancing for a shared memory system

Algorithm 1.7: *Load Balancing Based on Job Queue Management Scheme*

```
//Algorithm 12.7
// <data initialization>
// <loading the initial block pointer into the job queue>
// pick up the block from the job queue (if the job queue is not empty)
while ( (pBlock=GetBlock()) != NULL ) {
 // <block processing>
 // marking the neighboring block readiness for processing
 omp_set_lock(pBlock->pNext.Lock); // right-hand neighbor
    pBlock->pNext.Count++;
    if ( pBlock->pNext.Count == 2 )
      PutBlock(pBlock->pNext);
  omp_unset_lock(pBlock->pNext.Lock);
  omp_set_lock(pBlock->pDown.Lock); // lower neighbor
    pBlock->pDown.Count++;
    if ( pBlock->pDown.Count == 2 )
      PutBlock(pBlock->pDown);
  omp_unset_lock(pBlock->pDown.Lock);
} // the end of computations, as the queue is empty
```

Parallel Computations for Distributed Memory Systems

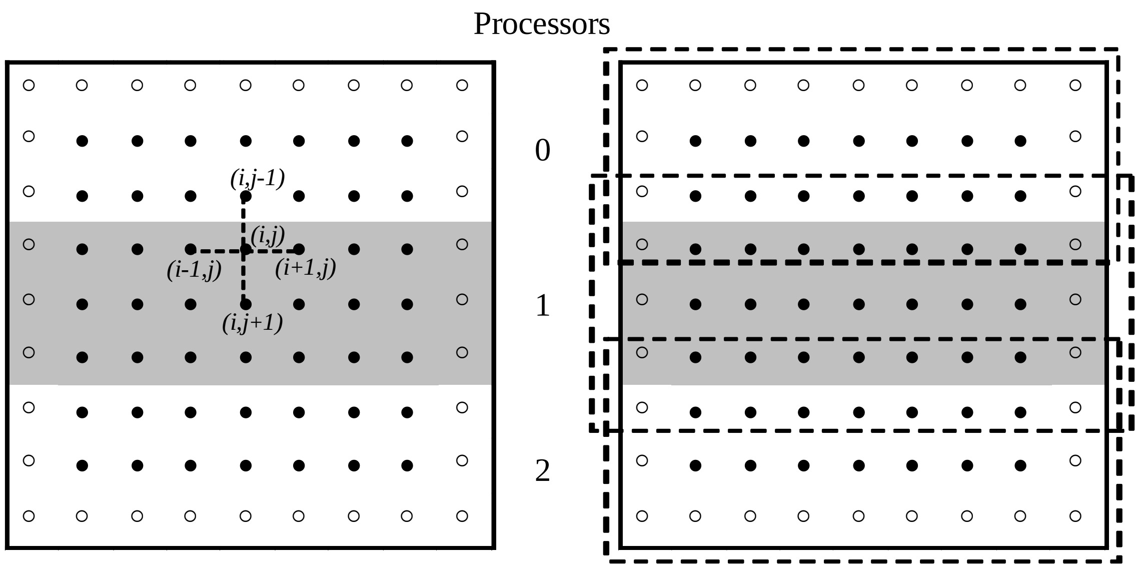
- Many parallel computation problems such as the race condition, deadlocks, serialization are common for the systems with shared and distributed memory
- The communication of parallel program parts on different processors can only be provided through *message passing*

Data Decomposition Schemes

- In the considered the Dirichlet problem there are two different data decomposition schemes:
  - The *one-dimensional* or *striped* decomposition of the domain grid,
  - The *two-dimensional* or *block-structured* (*checkerboard*) decomposition of the domain grid
- In case of striped decomposition the domain grid is divided into horizontal or vertical strips
- The number of strips is defined by the number of processors. The size of strips is usually equal
- The strips are distributed among the processors for processing

Striped Decomposition

- **Remarks:**
  - The border rows of the previous and the next strips should be copied on the processor, which performs processing a strip,
  - Border row copying should be performed prior to the beginning of the execution of each method iteration



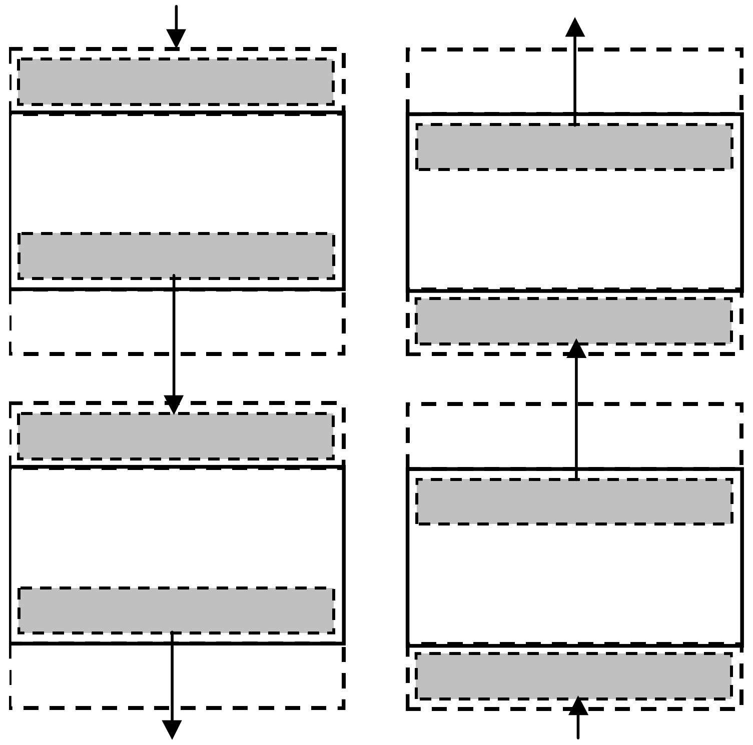
Algorithm 1.8: *The Gauss-Seidel Method, the Striped Data Decomposition*

```
// Algorithm 12.8
// The Gauss-Seidel method, the striped decomposition
// operations performed on each processor
do {
  // <border row exchange between the neighbors>
  // <strip processing>
  // <calculating the computational error dmax>
 while ( dmax > eps ); // eps – the required accuracy
```

Code

Data Distribution between Processors…

- At the first stage each processor transmits its lowest border row to the following processor and receives the analogous row from the previous processor
- At the second stage processors transmit their upper border rows to the previous neighbors and receive the analogous rows from the following neighbor



Data Distribution between Processors…

- Carrying out such data transmission operations may be implemented as follows:

```
// transmission of the lowest border row to the following
// processor and receiving the transmitted border row
// from the previous processor
if ( ProcNum != NP-1 )Send(u[M][*],N+2,NextProc);
if ( ProcNum != 0 )Receive(u[0][*],N+2,PrevProc);
```

- Such implemented scheme produces the ***strictly sequential execution*** of data transmission operations
- Applying *nonblocking* communications may not provide an efficient parallel scheme of processor interactions

Parallelization of Data Communications

- At the first step all odd processors transmit data, and the even processors receive the data
- At the second step the processors change their roles: the even processors perform the operation *Send*, the odd processors perform the operation *Receive*

```
// transmission of the lowest border row to the following processor
// and receiving the transmitted row from the previous processor
if ( ProcNum % 2 == 1 ) { // odd processor
if ( ProcNum != NP-1 )Send(u[M][*],N+2,NextProc);
  if ( ProcNum != 0 )Receive(u[0][*],N+2,PrevProc);
}
else { // even processor
  if ( ProcNum != 0 )Receive(u[0][*],N+2,PrevProc);
  if ( ProcNum != NP-1 )Send(u[M][*],N+2,NextProc);
}
```

Collective Communications

- Operation of accumulating and broadcasting the data may be implemented by the use of *the cascade scheme*
- Obtaining of the maximum value of local errors calculated by the processors may be provided by means of the following technique:
  – At the first step finding of the maximum values for pairwise grouped processor - such calculations may be performed at different processor pairs in parallel,
  – At the second step analogous pairwise calculations may be applied for finding the maximum values among the obtained results, etc.
- According with the cascade scheme it is necessary to perform $log_2 p$ of parallel iterations to calculate the total maximum value (p is the number of processors)

Algorithm 1.8: The Gauss-Seidel Method, Implementation with Collective Communication Operations

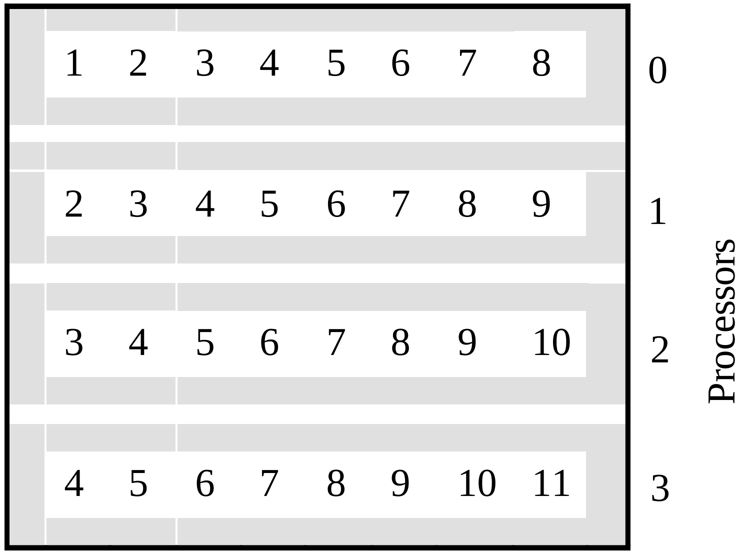
```
// Algorithm 12.8 – Implementation with Collective Operations
// The Gauss-Seidel method, the striped decomposition
// operations performed on each processor
do {
  // border strip row exchange with the neighbors
  Sendrecv(u[M][*],N+2,NextProc,u[0][*],N+2,PrevProc);
  Sendrecv(u[1][*],N+2,PrevProc,u[M+1][*],N+2,NextProc);
  // <strip processing with the error estimation dm >
  // <calculating the computational error dmax>
  Reduce(dm,dmax,MAX,0);
  Broadcast(dmax,0);
} while ( dmax > eps ); // eps – the required accuracy
```

The Results of Calculations Experiments

Grid size	Gauss-Seidel sequential method		Parallel algorithm 1.8		
	k	***T***	***k***	***T***	***S***
100	210	0,06	210	0,54	0,11
200	273	0,35	273	0,86	0,41
300	305	0,92	305	0,92	1,00
400	318	1,69	318	1,27	1,33
500	343	2,88	343	1,72	1,68
600	336	4,04	336	2,16	1,87
700	344	5,68	344	2,52	2,25
800	343	7,37	343	3,32	2,22
900	358	9,94	358	4,12	2,41
1000	351	11,87	351	4,43	2,68
2000	367	50,19	367	15,13	3,32
3000	364	113,17	364	37,96	2,98

Striped Wavefront Computations

- To form a wavefront calculations each strip can be represented logically as a set of blocks
- As a result of such logical structure the wavefront computation scheme may be executed. At the first step the block marked by the number 1 may be processed. Then – at the second step – the blocks marked by the number 2 may be recalculated, etc.



Block-structured (Checkerboard) Decomposition…

- In case of the block-structured (checkerboard) data decomposition the number of the border rows on each processor is increased, which leads correspondingly to a greater number of data communications in the border row transmission (but the number of transmitted elements is reduced)
- The use of the checkerboard scheme of data decomposition is appropriate if the number of grid nodes is essentially large

Block-structured (Checkerboard) Decomposition…

```
// Algorithm 12.9
// The Gauss-Seidel method, the striped decomposition
// operations executed on each processor
do {
  // obtaining border nodes
  if ( ProcNum / NB != 0 ) { // nonzero row of processors
    // obtaining data from upper processor
    Receive(u[0][*],M+2,TopProc); // upper row
    Receive(dmax,1,TopProc);      // computational error
  }
  if ( ProcNum % NB != 0 ) { // nonzero column of processors
    // obtaining data from left processor
    Receive(u[*][0],M+2,LeftProc); // left column
    Receive(dm,1,LeftProc);        // computational error
    If ( dm > dmax ) dmax = dm;
  }
```

Block-structured (Checkerboard) Decomposition

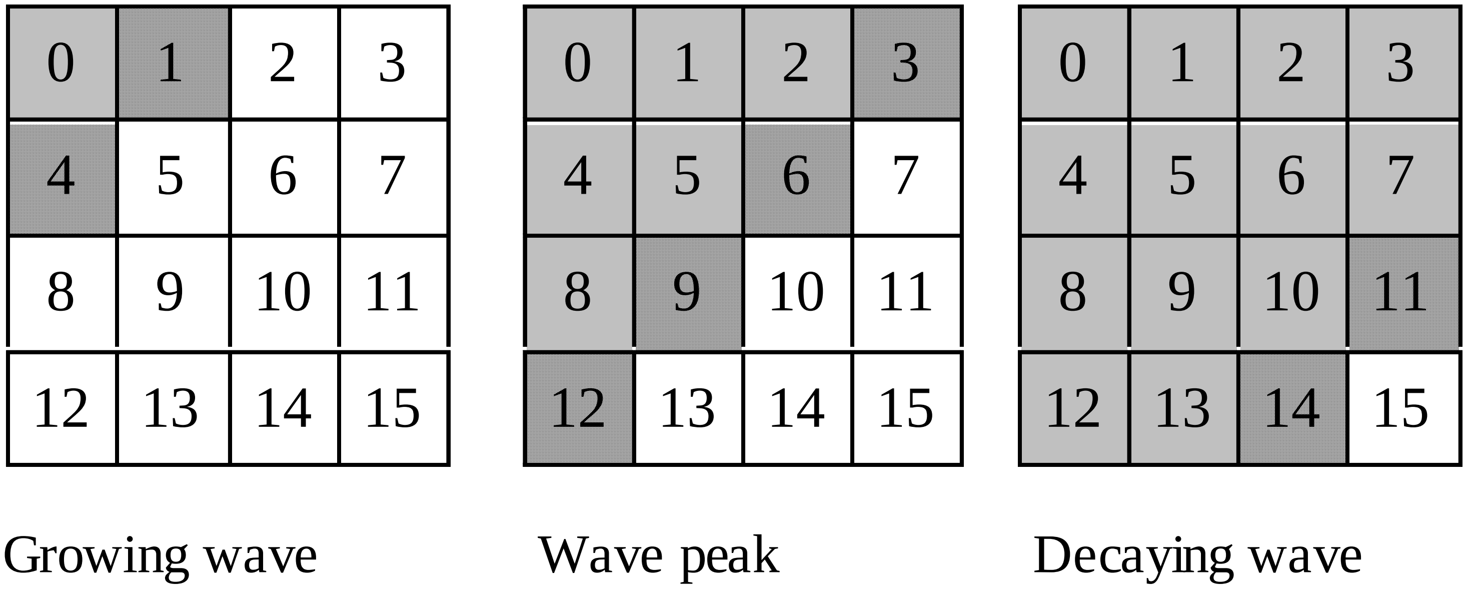
```
 // <processing a block with computational error dmax >
  // transmission of border nodes
  if ( ProcNum / NB != NB-1 ) { // processor row is not last
    //data transmission to the lower processor
    Send(u[M+1][*],M+2,DownProc); // bottom row
    Send(dmax,1,DownProc);        // computational error
  }
  if ( ProcNum % NB != NB-1 ) { // processor column is not last
     // data transmission to the right processor
     Send(u[*][M+1],M+2,RightProc); // right column
     Send(dmax,1, RightProc);       // computational error
  }
  // synchronization and distribution of the value dmax
  Barrier();
  Broadcast(dmax,NP-1);
} while ( dmax > eps ); // eps – the required accuracy
```

Code

Computational Pipelining (Multiple Wavefront Computation Scheme)…

- The wavefront computation efficiency decreases considerably because the processors perform calculations only at the moment when their blocks belongs to the wave computation front
- To improve the load balancing among the processors a *multiple wavefront computation scheme* can be applied
- The multiple wavefront method can be explained as follows: the processors may start processing the blocks of the following wave after executing the current calculation iteration

Computational Pipelining (Multiple Wavefront Computation Scheme)

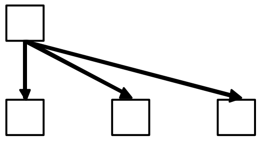
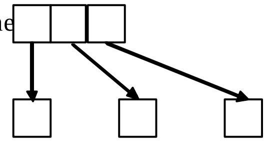
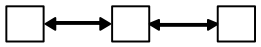
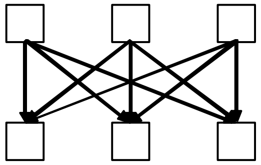
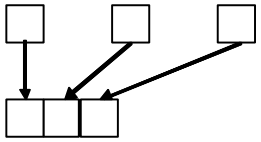


▨ blocks of the current iteration

☐ blocks of the previous iteration

■ blocks which nodes can be recalculated

Overview of Data Communications in Solving Partial Differential Equations

Communication operation	Processors 0 1 2	Corresponding MPI function
One-to-all distribution of the grid node number		MPI_Bcast
Scattering strips (blocks) of the grid nodes		MPI_Scatter
Exchanging borders of neighbor strips or blocks		MPI_Sendrecv
All-to-all calculating and distributing the computatinal error		MPI_Allreduce
Gathering strips (blocks) of the grid nodes		MPI_Gather

Summary

- The ways of parallel algorithm development for the systems with shared and distributed memory are discussed on the example of solving the partial differential equations
- In case of parallel computations on the systems with shared memory the main attention is given to the OpenMP technology; various aspects concerning with parallel programming are considered
- In case of parallel computations on the systems with distributed memory the problems of the data decomposition and the information communications between the processors are discussed; striped and checkerboard decomposition schemes are presented

Discussions

- What are the ways to increase the efficiency of wavefront methods?
- How can the job queue balance the computational load?
- What problems have to be solved in the process of parallel computation on distributed memory systems?
- What basic operations of data communications are used in the parallel methods of the Dirichlet problem?

Exercises

- Develop the parallel algorithm implementation of the wavefront computation scheme including the block-structured data decomposition scheme
- Develop theoretical estimation of the algorithm execution time
- Carry out the computational experiments. Compare the results of computational experiments and the obtained theoretical estimations

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Next Section

- Parallel Methods for Global Optimization

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About the project

The purpose of the project is to develop the set of educational materials for the teaching course “Multiprocessor computational systems and parallel programming”. This course is designed for the consideration of the parallel computation problems, which are stipulated in the recommendations of IEEE-CS and ACM Computing Curricula 2001. The educational materials can be used for teaching/training specialists in the fields of informatics, computer engineering and information technologies. The curriculum consists of **the training course “Introduction to the methods of parallel programming”** and **the computer laboratory training “The methods and technologies of parallel program development”**. Such educational materials makes possible to seamlessly combine both the fundamental education in computer science and the practical training in the methods of developing the software for solving complicated time-consuming computational problems using the high performance computational systems.

The project was carried out in Nizhny Novgorod State University, the Software Department of the Computing Mathematics and Cybernetics Faculty (http://www.software.unn.ac.ru). The project was implemented with the support of Microsoft Corporation.