

Iterative Solution of Sparse Equation Systems

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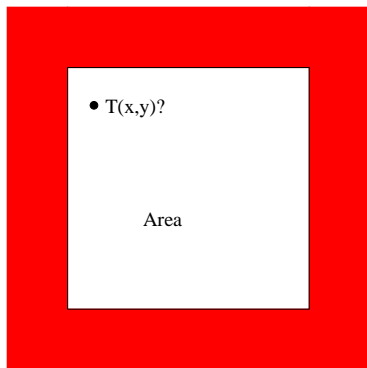
Iterative Solution of Sparse Linear Equation Systems

- Problem formulation
- Iteration methods
- Parallelisation
- Multigrid methods
- Parallelisation of multigrid methods

Problem Formulation: Example

A continuous problem and its discretisation:

- Example: A thin, quadratic metal plate is fixed at every side.
- The temporal constant temperature distribution at the boundary of the metal plate is known.
- Which temperature exists at each inner point of the metal plate, if the system is in a stationary state?



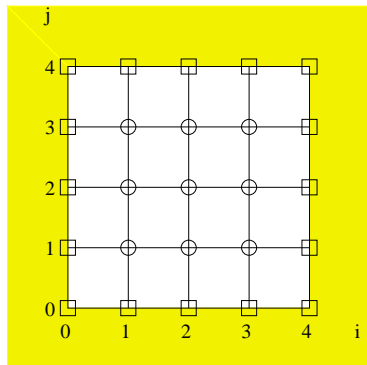
Problem Formulation: Continuous

- The process of heat conduction can be described (approximately) by a mathematical model.
- The geometry of the metal plate is described by an area $\Omega \subset \mathcal{R}^2$.
- Wanted is the temperature distribution $T(x, y)$ for all $(x, y) \in \Omega$.
- The temperature $T(x, y)$ for (x, y) on the boundary $\partial\Omega$ is known.
- Is the metal plate homogeneous (same heat conduction coefficient everywhere), then the temperature in the inner domain is described by the partial differential equation

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0, \quad T(x, y) = g(x, y) \text{ auf } \partial\Omega. \quad (1)$$

Problem Formulation: Discrete

- In the computer one cannot determine the temperature at every position $(x, y) \in \Omega$ (innumerable many), but only at some selected ones.
- For that be $\Omega = [0, 1]^2$ chosen specially (unit square).
- Via the parameter $h = 1/N$, for a $N \in \mathbf{N}$, we choose specially the points $(x_i, y_j) = (ih, jh)$, for all $0 \leq i, j \leq N$.
- One denotes this set of points also as regular, equidistant grid.



The points at the boundary have been marked with other symbols (squares) as the inner ones (circles).

Discretisation I

How can the temperature T_{ij} at point (x_i, y_j) be determined?

- By a standard method: the method of „Finite Differences“
- Idea: The temperature at point (x_i, y_j) is expressed by the values of the four neighboring points:

$$T_{i,j} = \frac{T_{i-1,j} + T_{i+1,j} + T_{i,j-1} + T_{i,j+1}}{4} \quad (2)$$

$$\iff T_{i-1,j} + T_{i+1,j} - 4T_{i,j} + T_{i,j-1} + T_{i,j+1} = 0 \quad (3)$$

für $1 \leq i, j \leq N - 1$.

- From the form of (3) one recognices, that all $(N - 1)^2$ equations for $1 \leq i, j \leq N - 1$ together form a linear equation system:

$$AT = b \quad (4)$$

Discretisation II

- Here $G(A)$ corresponds exactly to the above drawn grid, if one neglects the boundary points (squares). The righthand side b of (3) is not even zero, but contains the temperature values at the boundary!
- The such calculated temperature values $T_{i,j}$ at the points (x_i, y_j) are *not* identical with the solution $T(x_i, y_i)$ of the partial differential equation (1). Furthermore applies

$$|T_{i,j} - T(x_i, y_i)| \leq O(h^2) \quad (5)$$

- This error is denoted as „discretisation error“. An increase in the size of N corresponds such to an exacter temperature calculation.

Iteration Methods I

- We now want to solve the equation system (4) „iteratively“. Herefore we determine an arbitrary value of the temperature $T_{i,j}^0$ at each point $1 \leq i, j \leq N - 1$ (the temperature at the boundary is wellknown).
- Starting from this approximate solution we now want to calculate an improved solution. Herefore we use the formula (2) and set

$$T_{i,j}^{n+1} = \frac{T_{i-1,j}^n + T_{i+1,j}^n + T_{i,j-1}^n + T_{i,j+1}^n}{4} \quad \text{für alle } 1 \leq i, j \leq N - 1. \quad (6)$$

- Obviously the improved values $T_{i,j}^{n+1}$ can be calculated simultaneously for each of the indices (i, j) , since they only depend on the old values $T_{i,j}^n$.

Iteration Methods II

- One can indeed show, that

$$\lim_{n \rightarrow \infty} T_{i,j}^n = T_{i,j} \quad (7)$$

applies.

- The error $|T_{i,j}^n - T_{i,j}|$ in the n -th approximate solution is denoted as „iteration error“.
- How large is this iteration error then? One needs a criterium up to which n one needs to compute.

Iteration Methods III

- Herefore one considers how well the values $T_{i,j}^n$ fulfill the equation (3), this means we set

$$E^n = \max_{1 \leq i,j \leq N-1} |T_{i-1,j}^n + T_{i+1,j}^n - 4T_{i,j}^n + T_{i,j-1}^n + T_{i,j+1}^n|$$

- Commonly one uses this error only relatively, thus one iterates as long until

$$E^n < \epsilon E^0$$

applies. Then the initial error E^0 has been reduced by the reduction factor ϵ .

- This leads us to the sequential method:

choose N, ϵ ;

choose $T_{i,j}^0$;

$$E^0 = \max_{1 \leq i,j \leq N-1} |T_{i-1,j}^0 + T_{i+1,j}^0 - 4T_{i,j}^0 + T_{i,j-1}^0 + T_{i,j+1}^0|;$$

$n = 0$;

while ($E^n \geq \epsilon E^0$)

{

for ($1 \leq i, j \leq N - 1$)

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

$$E^{n+1} = \max_{1 \leq i,j \leq N-1} |T_{i-1,j}^{n+1} + T_{i+1,j}^{n+1} - 4T_{i,j}^{n+1} + T_{i,j-1}^{n+1} + T_{i,j+1}^{n+1}|;$$

$n = n + 1$;

}

Iteration Methods IV

- All that can be written more compact in vector notation. Then $AT = b$ is the equation system (4) to be solved. The approximation values $T_{i,j}^n$ correspond to vectors T^n each.
- Formally T^{n+1} is calculated as

$$T^{n+1} = T^n + D^{-1}(b - AT^n)$$

with the diagonal matrix $D = \text{diag}(A)$. This scheme is denoted as Jacobi method.

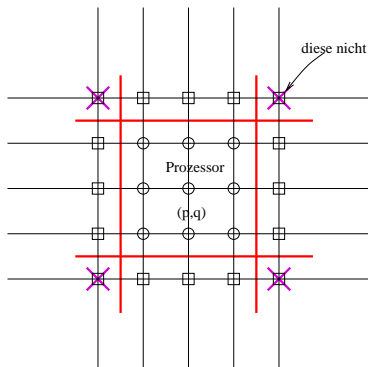
- The error E^n is constituted by

$$E^n = \|b - A \cdot T^n\|_{\infty},$$

where $\|\cdot\|_{\infty}$ is the maximum norm of a vector.

Parallelisation I

- The algorithm allows again a data parallel formulation.
- Therefore the $(N + 1)^2$ grid points are subdivided onto a $\sqrt{P} \times \sqrt{P}$ processor array by partitioning of the index set $I = \{0, \dots, N\}$.
- The partitioning happens here *block-wise*:



Parallelisation II

- Processor (p, q) computes then the values $T_{i,j}^{n+1}$ with $(i, j) \in \{start(p), \dots, end(p)\} \times \{start(q), \dots, end(q)\}$.
- To do this, he needs however also the values $T_{i,j}^n$ from the neighboring processors with $(i, j) \in \{start(p) - 1, \dots, end(p) + 1\} \times \{start(q) - 1, \dots, end(q) + 1\}$.
- These are the nodes, that have been marked with squares in the figure above!
- Each processor stores such beyond its assigned grid points an additional layer of grid points.

Parallelisation III

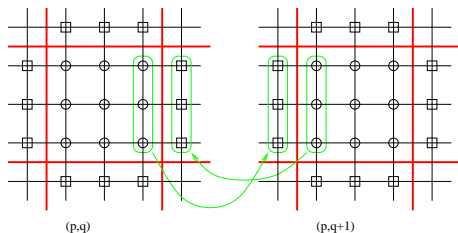
- The parallel algorithm therefore consists of the following steps:

initial values $T_{i,j}^0$ are known by all processors.

while ($E^n > \epsilon E^0$)

```
{  
  calculate  $T_{i,j}^{n+1}$  for  $(i,j) \in \{start(p), \dots, end(p)\} \times \{start(q), \dots, end(q)\}$ ;  
  exchange boundary values (squares) with neighbors;  
  calculate  $E^{n+1}$  for  $(i,j) \in \{start(p), \dots, end(p)\} \times \{start(q), \dots, end(q)\}$ ;  
  Determine global maximum;  
   $n = n + 1$ ;  
}
```

- In the exchange step two neighboring processors exchange values:



Parallelisation IV

- For this exchange step one uses either asynchronous communication or synchronous communication with coloration.
- We calculate the scalability of a *single* iteration:

$$W = T_S(N) = N^2 t_{op} \implies N = \sqrt{\frac{W}{t_{op}}}$$

$$T_P(N, P) = \underbrace{\left(\frac{N}{\sqrt{P}}\right)^2 t_{op}}_{\text{calculation}} + \underbrace{\left(t_s + t_h + t_w \frac{N}{\sqrt{P}}\right) 4}_{\text{boundary exchange}} + \underbrace{(t_s + t_h + t_w) \text{ld } P}_{\substack{\text{global} \\ \text{comm.: max.} \\ \text{for } E^n}}$$

$$T_P(W, P) = \frac{W}{P} + \frac{\sqrt{W}}{\sqrt{P}} \frac{4t_w}{\sqrt{t_{op}}} + (t_s + t_h + t_w) \text{ld } P + 4(t_s + t_h)$$

$$\begin{aligned} T_O(W, P) &= PT_P - W = \\ &= \sqrt{W}\sqrt{P} \frac{4t_w}{\sqrt{t_{op}}} + P \text{ld } P (t_s + t_h + t_w) + P4(t_s + t_h) \end{aligned}$$

Parallelisation V

- Asymptotically we obtain the iso-efficiency function $W = O(P \ln P)$ from the second term, albeit the first term will be dominant for practical values of N dominant. The algorithm is nearly optimal scalable.
- Because of the block-wise partitioning one has a surface-to-volume effect: $\frac{N}{\sqrt{P}} / \left(\frac{N}{\sqrt{P}}\right)^2 = \frac{\sqrt{P}}{N}$. In three space dimensions one obtains $\left(\frac{N}{P^{1/3}}\right)^2 / \left(\frac{N}{P^{1/3}}\right)^3 = \frac{P^{1/3}}{N}$.
- For same N and P the efficiency is such a little bit worse compared to two dimensions.

Multigrid Methods I

- If we ask about the total efficiency of a method, then the number of operations is distinctive.
- Hereby is

$$T_S(N) = IT(N) \cdot T_{IT}(N)$$

- How many iterationen have now indeed to be executed depends besides N of course on the used method.
- For that one obtains the following classifications:

$$\text{Jacobi, Gau\ss-Seidel : } IT(N) = \mathcal{O}(N^2)$$

$$\text{SOR with } \omega_{\text{opt}} : IT(N) = \mathcal{O}(N)$$

$$\text{Conjugated gradients (CG) : } IT(N) = \mathcal{O}(N)$$

$$\text{Hierarchical basis } d=2 : IT(N) = \mathcal{O}(\log N)$$

$$\text{Multigrid methods : } IT(N) = \mathcal{O}(1)$$

- The time for an iteration $T_{IT}(N)$ is there for all schemes in $\mathcal{O}(N^d)$ with comparable constant (in the region of 1 to 5).

Multigrid Methods II

- We such see, that e.g. the multigrid method is much faster than the Jacobi method.
- Also the parallelisation of the Jacobi method does not help, since it applies:

$$T_{P,\text{Jacobi}}(N, P) = \frac{\mathcal{O}(N^{d+2})}{P} \quad \text{und} \quad T_{S,\text{MG}}(N) = \mathcal{O}(N^d)$$

- A doubling of N results in a fourfold increase of the effort for the parallelised Jacobi scheme in comparison to the `sequential` multigrid method!
- This leads to a fundamental paradigm of parallel programming:

Parallelise the best sequential algorithm, if possible anyhow!

Multigrid Methods III

- Let us consider again the discretisation of the Laplace equation $\Delta T = 0$.
- This leads to the linear equation system

$$Ax = b$$

- Here the vector b is determined by the Dirichlet boundary values. Now be an approximation of the solution given by x^i . Herefore set the iteration error

$$e^i = x - x^i$$

- Because of the linearity of A we can conclude the following:

$$Ae^i = \underbrace{Ax}_b - Ax^i = b - Ax^i =: d^i$$

- Here we call d^i the defect.
- A good approximation for e^i is calculated by the solution of

$$Mv^i = d^i \quad \text{also} \quad v^i = M^{-1}d^i$$

- Herefore be M easier to solve than A (in $\mathcal{O}(N)$ steps, if $x \in \mathbb{R}^N$).

Multigrid Methods IV

- For special M we get the already known iteration method :

$$M = I \quad \rightarrow \text{Richardson}$$

$$M = \text{diag}(A) \quad \rightarrow \text{Jacobi}$$

$$M = L(A) \quad \rightarrow \text{Gau\ss-Seidel}$$

- We obtain the linear iteration method of the form

$$x^{i+1} = x^i + \omega M^{-1}(b - Ax^i)$$

- Here the $\omega \in [0, 1]$ is a damping factor .
- For the error $e^{i+1} = x - x^{i+1}$ applies:

$$e^{i+1} = (I - \omega M^{-1}A)e^i$$

- Here we denote the iteration matrix $I - \omega M^{-1}A$ with S .
- The scheme is exactly then convergent if applies ($\lim_{i \rightarrow \infty} e^i = 0$). This holds if the largest absolute eigen value of S is smaller than one.

Smoothing Property I

- If the matrix A is symmetric and positive definite, then it has only real, positive eigen values λ_k for eigen vectors z_k .
- The Richardson iteration

$$x^{i+1} = x^i + \omega(b - Ax^i)$$

leads because of $M = I$ to error

$$e^{i+1} = (I - \omega A)e^i$$

- Now we set the damping factor $\omega = \frac{1}{\lambda_{\max}}$ and consider $e^i = z_k (\forall k)$.
- Then we obtain

$$e^{i+1} = \left(I - \frac{1}{\lambda_{\max}} A \right) z_k = z_k - \frac{\lambda_k}{\lambda_{\max}} z_k = \left(1 - \frac{\lambda_k}{\lambda_{\max}} \right) e^i$$
$$\left(1 - \frac{\lambda_k}{\lambda_{\max}} \right) = \begin{cases} 0 & \lambda_k = \lambda_{\max} \\ \approx 1 & \lambda_k \text{ small } (\lambda_{\min}) \end{cases}$$

Smoothing Property II

- In the case of small eigenvalues we thus have a bad damping of the error (it has the order of magnitude of $1 - \mathcal{O}(h^2)$).
- This behaviour is qualitatively identical for the Jacobi and Gauß-Seidel iteration methods.
- But, to small eigenvalues belong long-wave eigenfunctions.
- This long-wave errors are such damped only very badly.
- With a pictorial view the iteration methods only offer a local smoothing of the error on which they work, since they get new iteration values only from values in the local neighborhood.
- Fast oscillations could be smoothed out fast, whilst long-wave errors survive the local smoothing operations quite unmodified.

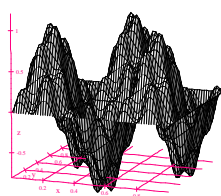
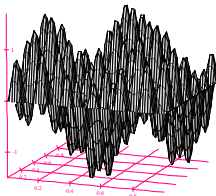
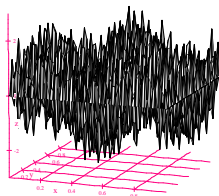
Smoothing Property III

For illustration purposes we consider the following example:

The Laplacian equation $-\Delta u = f$ is discretized via a five-point stencil on a structured grid. The associated eigenfunctions are $\sin(\nu\pi x) \sin(\mu\pi y)$, where $1 \leq \nu$ and $\mu \leq h^{-1} - 1$ apply. We set $h = \frac{1}{32}$ and the initial error to

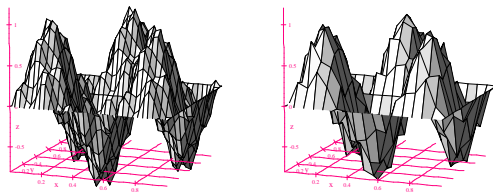
$$e^0 = \sin(3\pi x) \sin(2\pi y) + \sin(12\pi x) \sin(12\pi y) + \sin(31\pi x) \sin(31\pi y).$$

With $\omega = \frac{1}{\lambda_{\max}}$ one obtains the damping factors (per iteration) for the Richardson iteration as 0.984, 0.691 and 0 for the individual eigenfunctions. The graphs below show the initial error and the error after one resp. five iterations.



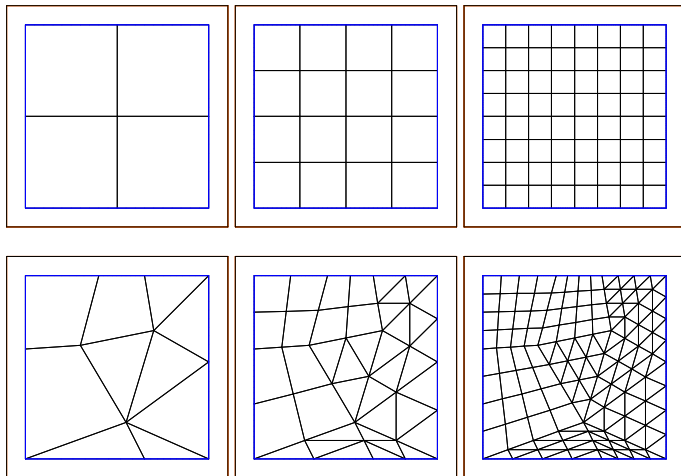
Smoothing Property IV

- From this the idea arises to represent the long wave error on coarser grids, after smoothing out the fast oscillations.
- On this coarser grids the effort is then smaller to smooth the error curve.
- Because the curve is somehow smooth after presmoothing, this restriction onto fewer grid points is well possible.



Grid Hierarchy I

- One constructs thus a complete sequence of grids of different accuracy.
- At first one smoothes out on the finest grid the short wave error functions.
- Then we restrict to the next coarser grid, and so on.



Grid Hierarchy II

- According to that one obtains a complete sequence of linear systems

$$A_l x_l = b_l,$$

since the number of grid points N and therefore the length of x decreases on coarser grids.

- Of course one wants to return after this restriction again to the original fine grid.
- Herefore we perform a coarse grid correction.
- Let us assume we are on grid level l , thus we consider the LES

$$A_l x_l = b_l$$

- On this level the iterate x_l^j is given with an error of e_l^j , thus the error equation

$$A e_l^j = b_l - A_l x_l^j$$

Lets suppose, x_l^j is the result of ν_1 Jacobi, Gauß-Seidel or similar iterations.

- Then e_l^j is relatively smooth and thus also properly representable on a coarser grid, this means it can be interpolated well from a coarser grid to a finer one.

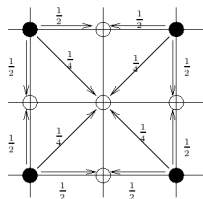
Grid Hierarchy III

- For this be v_{l-1} the error on the coarser grid.
- Then with good approximation applies

$$e_l^i \approx P_l v_{l-1}$$

- Here P_l is an interpolation matrix (prolongation), that performs a linear interpolation and changes the coarse grid vector into a fine grid vector.

1	0	0	0
$\frac{1}{2}$	$\frac{1}{2}$	0	0
0	1	0	0
$\frac{1}{2}$	0	$\frac{1}{2}$	0
$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$	$\frac{1}{4}$
0	$\frac{1}{2}$	0	$\frac{1}{2}$
0	0	1	0
0	0	$\frac{1}{2}$	$\frac{1}{2}$
0	0	0	1



Two-grid and Multigrid Methods I

- Through combination of the equations above one obtains the equation for v_{l-1} by

$$R_l A P_l v_{l-1} = R_l (b_l - A_l x_l^j)$$

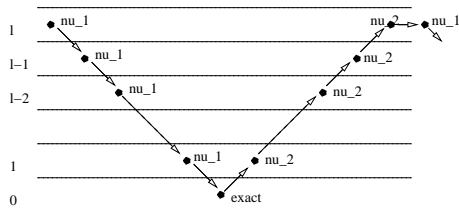
- Here is $R_l A P_l =: A_{l-1} \in \mathbb{R}^{N_{l-1} \times N_{l-1}}$ and R_l is the restriction matrix, for that one takes e.g. $R_l = P_l^T$.
- The so called two-grid method consists now of the two steps:
 - 1 ν_1 Jacobi iterations (on level l)
 - 2 coarse grid correction $x_l^{j+1} = x_l^j + P_l A_{l-1}^{-1} R_l (b_l - A_l x_l^j)$
- The recursive application leads to the multigrid methods.

`mgc(l, x_l, b_l)`

```
{  
    if (l == 0) x_0 = A_0^{-1} b_0;  
    else {  
        nu_1 iterations one-grid method on A_l x_l = b_l; // presmoothing  
        d_{l-1} = R_l (b_l - A_l x_l);  
        v_{l-1} = 0;  
        for (g = 1, ..., gamma)  
            mgc(l - 1, v_{l-1}, d_{l-1});  
        x_l = x_l + P_l v_{l-1};  
        nu_2 iterations one-grid method on A_l x_l = b_l; // postsmoothing  
    }  
}
```

Two-grid and Multigrid Methods II

- It is sufficient to set $\gamma = 1, \nu_1 = 1, \nu_2 = 0$ to get a iteration count of $\mathcal{O}(1)$.
- A single pass from level l to level 0 and back is denoted as V-cycle:



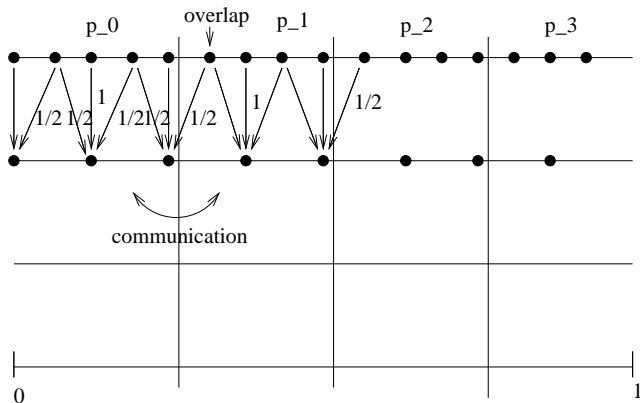
- Effort for two-dimensional structured grids: N is number of grid points in a row on the finest level, and $C := t_{op}$:

$$\begin{aligned}
 T_{IT}(N) &= \underbrace{CN^2}_{\text{level } l} + \underbrace{\frac{CN^2}{4}}_{\text{level } l-1} + \frac{CN^2}{16} + \dots + \underbrace{G(N_0)}_{\text{coarse grid}} \\
 &= CN^2 \left(1 + \frac{1}{4} + \frac{1}{16} + \dots \right) + G(N_0) = \frac{4}{3} CN_l + G(N_0)
 \end{aligned}$$

Parallelisation I

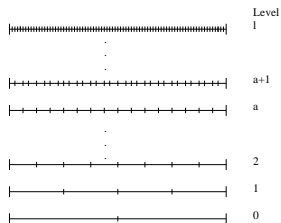
For data partitioning in the grid hierarchy on the individual processors one has to consider:

- In the coarse grid correction has to be checked, whether communication is necessary to calculate the node values in the coarse grid.
- How to handle the coarsest grids, where the number of unknowns in each dimension get smaller than the number of processors?



Parallelisation II

- For illustration of the method we only consider the one-dimensional case. The distribution in the high-dimensional case is according to the tensor product (chessboard-like).
- The processor limits are chosen at $p \cdot \frac{1}{P} + \epsilon$, such the nodes, that reside on the boundary between two processors, are still assigned to the „previous“.
- It is to remark, that the defect, that is restringated in the coarse grid correction, can only calculated on the single master node, but not in the overlap!
- To solve the problem with the decreasing node count in the coarsest grids, one uses successively fewer processors. Be for that $a := \text{Id } P$ and again $C := t_{\text{op}}$. On level 0 only one processor calculates, first on level a all are busy.



Parallelisation III

level	nodes	processors	effort
l	$N_l = 2^{l-a}N_a$	$P_l = P$	$T = 2^{l-a}CN_0$
$a+1$	$N_{a+1} = 2N_a$	$P_{a+1} = P$	$T = 2CN_0$
a	N_a	$P_a = P$	$T = CN_0$
2	$N_2 = 4N_0$	$P_2 = 4P_0$	$T = \frac{CN_2}{4} = CN_0$
1	$N_1 = 2N_0$	$P_1 = 2P_0$	$T = \frac{CN_1}{2} = \frac{C2N_0}{2} = CN_0$
0	N_0	$P_0 = 1$	$G(N_0) \stackrel{\text{be}}{\approx} CN_0$

- Let's consider the total effort: From level 0 to level a $\frac{N}{P}$ is constant, thus T_P grows like $\text{ld } P$. Therefore we get

$$T_P = \text{ld } P \cdot CN_0$$

- In the higher levels we get

$$T_P = C \cdot \frac{N_l}{P} \cdot \left(1 + \frac{1}{2} + \frac{1}{4} + \dots\right) = 2C \frac{N_l}{P}$$

- The total effort is then given by the sum of both partial efforts.
- Here we have not taken into account the communication between the processors.

Parallelisation IV

How effects the usage of the multigrid method the number of iteration steps to be executed?

- We show the number of used processors against the choice of the grid spacing, that has been used.
- The minimal error reduction has been set to 10^{-6} .

P/l	5	6	7	8
1	10			
4	10	10		
16	11	12	12	
64	13	12	12	12

- The table shows the according iteration times in seconds for 2D (factor 4 of grid growths):

P/l	5	6	7	8
1	3.39			
4	0.95	3.56		
16	0.32	1.00	3.74	
64	0.15	0.34	1.03	3.85

Most Important Knowledge

- Jacobi scheme is one of the most simple iteration methods for the solution of linear equation systems.
- For fixed reduction factor ϵ one necessitates a specific number of iterations IT to reach a certain error reduction.
- IT is *independent* on the choice of the starting value, but depends directly from the choice of the method (e.g. Jacobi scheme) and the grid spacing h (thus N).
- For the Jacobi method applies $IT = O(h^{-2})$. For a halvening of the grid width h one needs the fourfold number of iterations to get the error reduction ϵ . Since an iteration costs also four times more, the effort has increased by a factor of 16!
- There are a series of better iteration schemes for which e.g. $IT = O(h^{-1})$, $IT = O(\log(h^{-1}))$ or even $IT = O(1)$ applies (CG method, hierarchical basis, multigrid method).
- Of course asymptotically ($h \rightarrow \infty$) each of these methods is superior to a parallel naive scheme.
- One should therefore at all parallelize the method with optimal sequential complexity, especially because we want to solve large problems (h small) on parallel machines.