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HIERARCHICAL GRID COARSENING FOR THE SOLUTION OF THE POISSON EQUATION IN FREE SPACE*

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Abstract. In many applications the solution of PDEs in infinite domains with vanishing boundary conditions at infinity is of interest. If the Green's function of the particular PDE is known, the solution can easily be obtained by folding it with the right hand side in a finite subvolume. Unfortunately this requires $\mathcal{O}(N^2)$ operations. Washio and Oosterlee presented an algorithm that rather than that uses hierarchically coarsened grids in order to solve the problem (Numer. Math. (2000) 86: 539–563). They use infinitely many grid levels for the error analysis. In this paper we present an extension of their work. Instead of continuing the refinement process up to infinitely many grid levels, we stop the refinement process at an arbitrary level and impose the Dirichlet boundary conditions of the original problem there. The error analysis shows that the proposed method still is of order h^2, as the original method with infinitely many refinements.

Key words. the Poisson equation, free boundary problems for PDE, multigrid method

AMS subject classifications. 35J05, 35R35, 65N55

1. Introduction. Applications such as flow simulations around aircrafts (c.f. [4]) and molecular dynamics simulations (see [8]) require so-called free or open boundary conditions. Consider for example the Poisson equation with vanishing boundary conditions at infinity

$$\begin{aligned} \Delta u(\mathbf{x}) &= f(\mathbf{x}),\ \mathbf{x} \in \mathbb{R}^3, \\ u(\mathbf{x}) &\to 0,\ ||\mathbf{x}|| \to \infty, \end{aligned}$$

where supp(f) is a bounded subset of $\mathbb{R}^3$, as needed in molecular dynamics simulations to calculate the interaction between charges due to the electrostatic potential.

This problem has a discrete analog. Let Δ_h be a discretization of the Laplace operator on a infinite regular grid with mesh-width h. Then the infinitely large system of equations given by

$$\begin{aligned} \Delta_h u(\mathbf{x}) &= f(\mathbf{x}),\ \mathbf{x} \in \{\mathbf{x} \mid \mathbf{x} = h\,\mathbf{z}, \mathbf{z} \in \mathbb{Z}^3\}, \\ u(\mathbf{x}) &\to 0,\ ||\mathbf{x}|| \to \infty \end{aligned}$$

is the discretization of the continous problem.

There are different approaches to solve the discrete problem. We just want to mention a few of them:

1. Solution in a finite subvolume by explicitly imposing boundary values.
2. Solving the problem on a hierarchically coarsened infinitely large grid.
3. Solution of the problem on a hierarchically coarsened finite grid by imposing boundary values.

The first approach was chosen by Buneman in [3] to solve a two-dimensional potential problem. He derived a recursive formula for the discrete Green's function, i.e., a function G_h which satisfies

$$\Delta_h G_h(\mathbf{x}, \mathbf{y}) = \delta_h(\mathbf{x}, \mathbf{y}),$$

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where δ_h is the discrete Dirac-δ. This yielded an exact solution of the discrete problem, i.e. a solution of the continuous problem that is only disturbed by the discretization error of Δ_h. Later on in [4], Burkhart derived an asymptotic expansion of the discrete Green's function in $\mathbb{R}^3$ that allows the same proceedure for the three-dimensional case. This asymptotic expansion is given by

$$G_h(\mathbf{x}) = \frac{1}{4\pi}\left[\frac{1}{||\mathbf{x}||_2} + \frac{\eta_3}{||\mathbf{x}||_2^3} + \frac{\eta_5}{||\mathbf{x}||_2^5} + \dots\right],$$

where $\eta_i = \mathcal{O}(h^2)$.

Unfortunately these proceedures share the high computational costs of imposing the Dirichlet boundary conditions explicitly by using the recursive formula or the asymptotic expansion. Consider a cube with $N^{1/3}$ grid points in each direction. In order to compute the values at all boundary points, the formula or the expansion has to be evaluated

$$6N\left(N^{\frac{1}{3}}\right)^2 = 6N^{\frac{5}{3}}$$

times. So the overall complexity is polynomial with exponent $5/3$, which is unsatisfying when one uses an optimal, i.e. $\mathcal{O}(N)$, Poisson solver.

When dealing with particle systems, this problem can be avoided by using a multipole expansion in order to evaluate the potential on the boundary, as proposed by Sutmann and Steffen in [8].

The second approach was introduced by Washio and Oosterlee in [9]. They introduced a hierarchical grid coarsening, which uses the idea of locally refined grids, in order to reduce the computational cost outside of the subdomain of interest. They do this by extending the original grid hierarchically by a factor α, while coarsening the grid at the same time. They have shown that the result of this process is accurate to order h^2, if $\alpha > 2^{2/3}$. For their numerical experiments, they have chosen to stop the process after a number of steps and impose Dirichlet zero boundary conditions there.

In this paper we have extended their work imposing Dirichlet boundary conditions of the continuous problem at the level at which we stop the refinement. Since the number of boundary points is dramatically reduced, our method does not suffer from the computational cost of imposing the boundary values as described in [4] or similar approaches.

In the following the hierarchical grid coarsening will be explained in detail, followed by the appropriate extension of Washio's and Oosterlee's error analysis and some numerical experiments.

2. Solution using hierarchical grid coarsening. Assuming that we are interested in the solution of

$$\Delta u(\mathbf{x}) = f(\mathbf{x}),\ \mathbf{x} \in \mathbb{R}^3,$$
$$u(\mathbf{x}) \to 0,\ ||\mathbf{x}|| \to \infty,$$

inside of $\Omega = [-\frac{1}{2}, \frac{1}{2}]^3$, where $\mathrm{supp}(f) \subset \Omega$. In order to do so, we are discretizing Ω using a regular grid with mesh-width h and Δ using the standard 7-point discretization Δ_h.

2.1. Extension of the grid. The original grid is extended with the help of a grid extension rate $\alpha \in (1, 2)$ in the following way: The grid on the finest level is defined to be the

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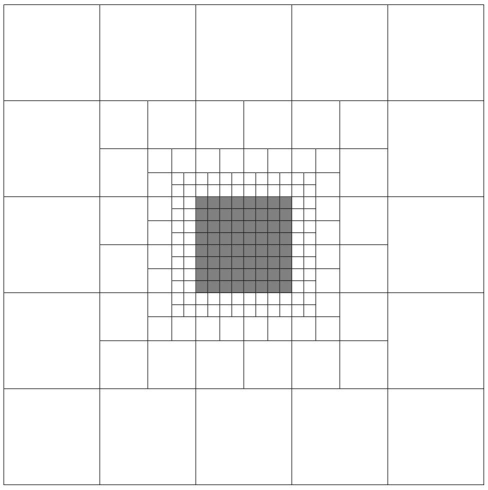

FIG. 2.1. *Coarsened grid in 2D. Highlighted is the original fine grid, in which the solution is of interest.*

discretization of domain Ω_1 with grid-width h_1, where

$$\begin{aligned} \Omega_1 &:= \left[-\frac{\beta_1}{2}, \frac{\beta_1}{2}\right]^3, \\ \beta_1 &\geq \alpha, \\ h_1 &:= h. \end{aligned}$$

So Ω_1 is just an extension of the original domain Ω. The domain is then extended and the grid is coarsened up to a level $l_{\max}$ as

$$\begin{aligned} \Omega_l &:= \left[-\frac{\beta_l}{2}, \frac{\beta_l}{2}\right]^3, \\ \beta_l &\geq \alpha^l, \\ h_l &:= 2^{(l-1)}\ h. \end{aligned}$$

The additional parameters β_l are introduced in order to enable the extended grids to have common grid points with the fine grids. Furthermore we define the set of grid points $\mathcal{G}_l$ on level l to be

$$\mathcal{G}_l := \{\, \mathbf{x} \in \Omega_l \ |\mathbf{x} = \ h_l\, \mathbf{z}, \mathbf{z} \in \mathbb{Z}\,\}\,.$$

An example of how a coarsened grid might look like in 2-D can be found in Fig. 2.1.

2.2. Setting boundary conditions. At the boundary of $\Omega_{l_{\max}}$ Dirichlet boundary conditions derived from the continous problem are imposed, i.e.,

$$u(\mathbf{x}_\partial) = \frac{1}{4\pi} \int\limits_\Omega \frac{f(\mathbf{x})}{||\mathbf{y} - \mathbf{x}_\partial||_2} d\mathbf{y},\ \forall\, \mathbf{x}_\partial \in \partial\Omega_{l_{\max}}.$$

2.3. Conservative discretization at the interface. To solve the problem on the composite grid

$$\mathcal{G} := \mathcal{G}_1 \cup \mathcal{G}_2 \cup \cdots \cup \mathcal{G}_{l_{\max}},$$

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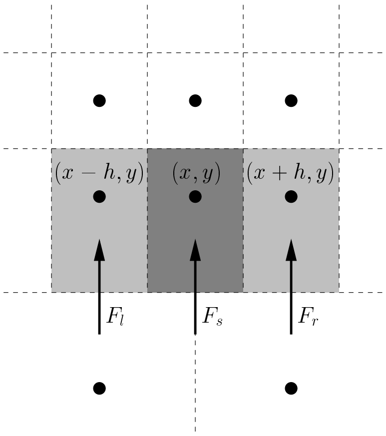

FIG. 2.2. *Conservative discretization at the interface in 2D.*

a discretization has to be chosen at the interfaces between Ω_l and $\Omega_{l+1} \backslash \Omega_l$. In order to obtain good approximation properties, it is vital to require this discretization to be conservative. A simple conservative discretization is the finite volume discretization using cubes around the grid points.

As an example consider the two-dimensional discretization using finite volumes at the refinement boundary depicted in Fig. 2.2 (the extension to 3-D is straightforward):

If we integrate the Poisson equation in a volume V and apply Gauß's divergence theorem, we get

$$\begin{aligned} \int_V \Delta u(\mathbf{x}) d\mathbf{x} &= \int_V f(\mathbf{x}) d\mathbf{x} \\ \Leftrightarrow \oint_{\partial V} \nabla u(\mathbf{s}) \cdot \vec{n}\, d\mathbf{s} &= \int_V f(\mathbf{x}) d\mathbf{x}. \end{aligned}$$

For the rectangular elements we have to deal with, this equation can be approximated by the sum of the fluxes times the length of the corresponding sides on the left hand side and by the value at the center times the area of the element on the right hand side. The fluxes are approximated using finite differences.

For square elements this coincides with the standard 5-point approximation of the Laplace operator times h^2, but we also have to deal with the elements on the boundary. The fine elements which have only one coarse neighbour are easy to treat, as the flux can directly be approximated by the finite difference. The flux at the border of two coarse elements of a fine element is the linear interpolation of the two neighbouring fluxes. So the flux F_s in Fig. 2.2 is just set to

$$F_s = \frac{1}{2}(F_l + F_r).$$

2.4. Solution of the resulting system of linear equations. Any solver can be used to solve the resulting linear system, but a multigrid method is particularly well suited to solve this problem, as it directly benefits from the structure of the composite grid $\mathcal{G}$. On each level of the multigrid cycle only the grid points contained in the corresponding region are treated, i.e., at level l only the points in $\mathcal{G}_l$ have to be taken into account. The information from the

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whole problem is being transfered to this level by interpolation and through smoothing, as the smoother uses information from Ω_{l+1} when smoothing the boundary points of Ω_l. The resulting method is based on McCormick's FAC (see [5, 6, 7]) and is given by:

Algorithm 1 FAC method for the solution of the resulting linear system.

$$\mathbf{u}_k \leftarrow \text{smooth}^{\nu_1}(\mathbf{u}_k)$$
$$\mathbf{d}_k \leftarrow \mathbf{f}_k - L_{h_k}\mathbf{u}_k$$
$$\mathbf{d}_{k+1} \leftarrow I_k^{k+1}\mathbf{d}_k$$
$$\mathbf{u}_{k+1} \leftarrow \begin{cases} \hat{I}_k^{k+1}\mathbf{u}_k, & \mathbf{u}_{k+1} \in \Omega_{k+1} \cap \Omega_k \\ \mathbf{u}_{k+1}, & \mathbf{u}_{k+1} \in \Omega_{k+1} \backslash \Omega_k \end{cases}$$
$$\mathbf{f}_{k+1} \leftarrow \begin{cases} \mathbf{d}_{k+1} + L_{k+1}\mathbf{u}_{k+1}, & \mathbf{u}_{k+1} \in \Omega_{k+1} \cap \Omega_k \\ \mathbf{f}_{k+1}, & \mathbf{u}_{k+1} \in \Omega_{k+1} \backslash \Omega_k \end{cases}$$
$$\mathbf{v}_{k+1} \leftarrow L_{k+1}^{-1}\mathbf{f}_{k+1} - \mathbf{u}_{k+1}$$
$$\mathbf{v}_k \leftarrow I_{k+1}^k \mathbf{v}_{k+1}$$
$$\mathbf{u}_k \leftarrow \mathbf{u}_k + \mathbf{v}_k$$
$$\mathbf{u}_k \leftarrow \text{smooth}^{\nu_2}(\mathbf{u}_k)$$

This is a slight modification of the work of Washio and Oosterlee [9], who used Brandt's MLAT (cf. [1, 2]) and incorporated the conservative discretization at the boundary through a conservative interpolation there.

2.5. Summary. The proposed modified method calculates the discrete solution of the Poisson equation inside of the unit square due to a right hand side f, where the support of f is a subset of the unit square. The method can be summarized as follows:

1. Choose grid extension rate $\alpha \in (0, 2)$ and maximum number of refinement steps $l_{\max}$.
2. Generate grid hierarchy $\mathcal{G}_l, l = 1, 2, \ldots, l_{\max}$, discretizing the appropriate domains Ω_l with mesh-widths h_l.
3. Set boundary values on the boundary points of the coarsest grid $\mathcal{G}_{l_{\max}}$ to the values derived from the continous problem.
4. Determine the composite grid $\mathcal{G}$ containing all grid points from all levels, using a conservative discretization scheme for the Laplace operator.
5. Solve the resulting system of linear equations.

3. Error analysis. For the error analysis, we start with a formal definition of the discrete and the cell-averaged Green's function.

DEFINITION 3.1 (Discrete Green's function). *Let Δ_h be a discretization of the Laplace operator on the grid $\{\, \mathbf{x} \mid \mathbf{x} = h\,\mathbf{z}, \mathbf{z} \in \mathbb{Z}^3\}$ and let $\delta_h(\mathbf{x}, \mathbf{y})$ be defined as*

$$\delta_h(\mathbf{x}, \mathbf{y}) := \begin{cases} 1, & \mathbf{x} = \mathbf{y} \\ 0 & \textit{otherwise} \end{cases} .$$

Then the discrete Green's function is defined by

$$\Delta_h G_h(\mathbf{x}, \mathbf{y}) := \delta_h(\mathbf{x}, \mathbf{y}),$$

where Δ_h is w.r.t. the first argument $\mathbf{x}$, only.

DEFINITION 3.2 (Cell-averaged Green's function). *Let $G(\mathbf{x}, \mathbf{y})$ be the Green's function of the Laplace operator Δ and let $\Omega_{\mathbf{x}}$ be defined as the cube with volume h^3 centered at $\mathbf{x}$, i.e.,*

$$\Omega_{\mathbf{x}} := \left\{ \mathbf{y} \;\middle|\; ||\mathbf{x} - \mathbf{y}||_\infty \le \frac{h}{2} \right\}.$$

The cell-averaged Green's function $\tilde{G}$ is given by

$$\tilde{G}(\mathbf{x},\mathbf{y}) = \frac{1}{h^3}\int\limits_{\Omega_{\mathbf{x}}} G(\mathbf{z},\mathbf{y})d\mathbf{z}.$$

As we chose a conservative discretization, Green's identity holds for the discrete case as well. Thus we obtain

$$\int\limits_{\Omega}[u(\Delta_h v) - (\Delta_h u)v]\,d\mathbf{x} = \oint\limits_{\partial\Omega}[u(\nabla_h v) - (\nabla_h u)v]\cdot\vec{\mathbf{n}}\,d\mathbf{s}.$$

Therefore, for the discrete Green's function G_h, it holds true that

$$\int\limits_{\Omega} G_h(\mathbf{x},\mathbf{y})[-\Delta\Psi_h(\mathbf{y})]\,d\mathbf{y} =$$

$$\Psi_h(\mathbf{x}) - \oint\limits_{\partial\Omega}[G_h(\mathbf{x},\mathbf{s})(\nabla_h\Psi_h(\mathbf{s})) - (\nabla_h G_h(\mathbf{x},\mathbf{s}))\Psi_h(\mathbf{s})]\cdot\vec{\mathbf{n}}\,d\mathbf{s}. \tag{3.1}$$

With this observation, we are now ready to provide an error analysis for our modification.

THEOREM 3.3. *Using the described grid coarsening strategy up to an arbitrary level while imposing Dirichlet boundary conditions derived from the continuum problem at the boundary of the coarsest grid, using a grid extension rate $\alpha \geq 2^{2/3}$ and under the assumption that*

$$G_h(\mathbf{x},\mathbf{p}) \leq \frac{1}{4\pi}\left[\frac{1}{||\mathbf{x}-\mathbf{p}||_2} + \frac{c_1}{||\mathbf{x}-\mathbf{p}||_2^3}\right],$$

the error $e(\mathbf{x},\mathbf{p})$, defined as

$$e(\mathbf{x},\mathbf{p}) := |\tilde{G}(\mathbf{x},\mathbf{p}) - G_h(\mathbf{x},\mathbf{p})|,$$

is of order h^2 for all $\mathbf{x} \in \mathcal{G}_0$.

Proof. We start by applying the discrete version of Green's identity, inserting $e(\mathbf{x},\mathbf{p})$ into (3.1) and get

$$e(\mathbf{x},\mathbf{p}) = \Bigg| \int\limits_{\Omega_{l_{\max}}} G_h(\mathbf{x},\mathbf{y})[-\Delta_h(\tilde{G}(\mathbf{y},\mathbf{p}) - G_h(\mathbf{y},\mathbf{p}))]\,d\mathbf{y} +$$

$$\oint\limits_{\partial\Omega_{l_{\max}}}\Big[G_h(\mathbf{x},\mathbf{s})\nabla_h(\tilde{G}(\mathbf{s},\mathbf{p}) - G_h(\mathbf{s},\mathbf{p})) - \nabla_h G_h(\mathbf{x},\mathbf{s})(\tilde{G}(\mathbf{s},\mathbf{p}) - G_h(\mathbf{s},\mathbf{p}))\Big]\cdot\vec{\mathbf{n}}\,d\mathbf{s}\Bigg|$$

For an estimate of the first integral, we make use of the excellent work of Washio and Oosterlee [9]. It is well known that the accuracy of the solution on the finest grid is of order h^2. So the error due to the integration over the finest grid is bounded by

$$|e_0(\mathbf{x},\mathbf{p})| \leq c_0 h^2.$$

Washio and Oosterlee showed that the error e_1 due to the region outside the finest grid, but not including the non-cubic-cells is bounded by

$$|e_1(\mathbf{x},\mathbf{p})| \leq c_1\frac{\alpha^3-1}{1-2^2/\alpha^3}\frac{h^2}{d_{\mathbf{x}}d_{\mathbf{p}}^5}$$

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and that the error e_2 due to the non-cubic cells is bounded by

$$|e_2(\mathbf{x}, \mathbf{p})| \leq c_2 \frac{1}{1 - 2^2/\alpha^3} \frac{h^2}{d_{\mathbf{x}} d_{\mathbf{x}}^4},$$

where $d_{\mathbf{x}}$ and $d_{\mathbf{p}}$ are the minimum distances from the boundary of the finest grid of $\mathbf{x}$ and $\mathbf{p}$, respectively. The proof depends on the fact that there exist constants $c_k(k = 0, 1, 2, \ldots)$, such that

$$|\Delta_y^{k-m} \Delta_p^m G(\mathbf{y}, \mathbf{p})| \leq \frac{c_k}{|\mathbf{y} - \mathbf{p}|^{k+1}}, (m \leq k),$$

where Δ_y and Δ_p act on $\mathbf{y}$ and $\mathbf{p}$, respectively. For further details we refer to [9]. Overall, the first integral can be bounded as follows:

$$\left| \int\limits_{\Omega_{l_{\max}}} G_h(\mathbf{x}, \mathbf{y})[-\Delta_h(\tilde{G}(\mathbf{y}, \mathbf{p}) - G_h(\mathbf{y}, \mathbf{p}))] \, d\mathbf{y} \right| \leq e_0 + e_1 + e_2 = \mathcal{O}(h^2).$$

It remains to show, that the second integral is bounded by an order h^2 term as well, i.e., that the setting of the boundary values to the ones derived from the continuous problem induces an error of order h^2. Let therefore d be the minimum distance of a point of the original domain to the boundary of the domain discretized using the coarsest grid. As both, $\mathbf{x}$ and $\mathbf{p}$ are inside of the original domain, we can bound the second integral,

$$\begin{aligned}
&\left| \oint\limits_{\partial\Omega_{l_{\max}}} \left[G_h(\mathbf{x}, \mathbf{s}) \nabla_h (\tilde{G}(\mathbf{s}, \mathbf{p}) - G_h(\mathbf{s}, \mathbf{p})) - \nabla_h G_h(\mathbf{x}, \mathbf{s})(\tilde{G}(\mathbf{s}, \mathbf{p}) - G_h(\mathbf{s}, \mathbf{p})) \right] \cdot \vec{\mathbf{n}} \, d\mathbf{s} \right| \\
&\quad \leq \alpha^{3l_{\max}} \max_{\mathbf{s} \in \partial\Omega_{l_{\max}}} \left[\left| G_h(\mathbf{x}, \mathbf{s}) \nabla_h (\tilde{G}(\mathbf{s}, \mathbf{p}) - G_h(\mathbf{s}, \mathbf{p})) \cdot \vec{\mathbf{n}} \right| + \right. \\
&\qquad\qquad \left. \left| \nabla_h G_h(\mathbf{x}, \mathbf{s}) \cdot \vec{\mathbf{n}} \, (\tilde{G}(\mathbf{s}, \mathbf{p}) - G_h(\mathbf{s}, \mathbf{p})) \right| \right] \\
&\quad \leq \alpha^{3l_{\max}} \left[\left(\left| \frac{1}{4\pi} \frac{1}{d} \right| + \left| \frac{c_1 h_{l_{\max}}^2}{d^3} \right| \right) \left| \frac{3c_1 h_{l_{\max}}^2}{d^4} \right| + \left(\left| \frac{1}{4\pi} \frac{1}{d^2} \right| + \left| \frac{3c_1 h_{l_{\max}}^2}{d^4} \right| \right) \left| \frac{c_1 h_{l_{\max}}^2}{d^3} \right| \right] \\
&\quad = \alpha^{3l_{\max}} \left[\left| \frac{1}{4\pi} \frac{3c_1 h_{l_{\max}}^2}{d^5} \right| + \left| \frac{3c_1^2 h_{l_{\max}}^4}{d^6} \right| + \left| \frac{1}{4\pi} \frac{3c_1 h_{l_{\max}}^2}{d^6} \right| + \left| \frac{3c_1^2 h_{l_{\max}}^4}{d^7} \right| \right].
\end{aligned}$$

Obviously, for $\alpha \geq 2^{2/3}$ we can bound d by

$$d = \frac{\alpha^l - 1}{2} \geq \frac{\alpha^l}{4}$$

and for $h_{l_{\max}}$ we have

$$h_{l_{\max}} = 2^{(l-1)} h_1 = 2^{(l-1)} h.$$

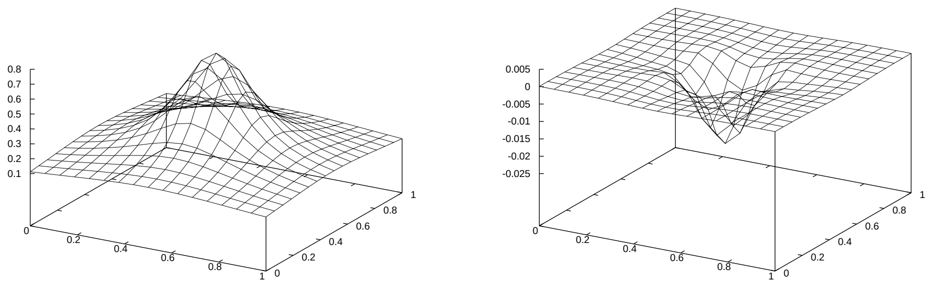

FIG. 4.1. *A cut through the computed solution of the test case (left) and its point-wise error (right).*

So we get

$$\alpha^{3l_{\max}}\left[\left|\frac{1}{4\pi}\frac{3c_1h_{l_{\max}}^2}{d^5}\right|+\left|\frac{3c_1^2h_{l_{\max}}^4}{d^6}\right|+\left|\frac{1}{4\pi}\frac{3c_1h_{l_{\max}}^2}{d^6}\right|+\left|\frac{3c_1^2h_{l_{\max}}^4}{d^7}\right|\right]$$
$$\leq \alpha^{3l_{\max}}\left[\left|\frac{1}{4\pi}\frac{3072c_1h^2}{\alpha^5}\left(\frac{2^2}{\alpha^5}\right)^{(l-1)}\right|+\left|\frac{12288c_1^2h^4}{\alpha^6}\left(\frac{2^4}{\alpha^6}\right)^{(l-1)}\right|+\right.$$
$$\left.\left|\frac{1}{4\pi}\frac{12288c_1h^2}{\alpha^6}\left(\frac{2^2}{\alpha^6}\right)^{(l-1)}\right|+\left|\frac{49152c_1^2h^4}{\alpha^7}\left(\frac{2^4}{\alpha^7}\right)^{(l-1)}\right|\right].$$

This is order h^2 for $\alpha > 2^{2/3}$. □

4. Numerical tests. The method has been implemented in C and tested to check the theoretical results. The performance was measured on a machine with an 1.7 GHz Power4+ CPU. The grid extension rate α was set to $1.6 > 2^{2/3}$ and for practical reasons β has been chosen as

$$\beta := \lceil 2^{\lceil \log_2(\alpha^l)\rceil}\rceil.$$

We used a cubic B-spline at the center of our domain of interest as the right hand side. So the exact solution u^* to the problem is known analytically.

In Fig. 4.1 the computed solution of our test case and its error are shown. We calculated the solution of the Poisson equation in free space for to a point-symmetric right hand side, which can be described by a B-spline and which has unit volume on a 17^3 grid. The error behaves as expected: It is very similar to the solution of the problem with explicitly set Dirichlet boundary conditions on the boundary of the computational box, but the error is not exactly zero on the boundary. Table 4.1 gives the norm of the error and timings for different grid sizes. One sees that the method scales linearly and the ∞-norm of the error decreases as expected.

In order to show that the number of refinement steps makes no difference with respect to the method's accuracy, we have tested the method using a different number of refinement steps. The results of these tests can be found in Table 4.2. The norm of the error does not change very much when the number of the refinement steps is varied, but of course the timings differ a lot, as the number of boundary points is dramatically reduced and the size of the linear system on the coarsest level as well.

TABLE 4.1
Error and timings for different various sizes. The ∞-norm of the error decreases as predicted and the method scales linearly with the number of grid points.

$\#\mathcal{G}_0$	h	#refinements	$\|\|\mathbf{u}-\mathbf{u}^*\|\|_\infty$	$\|\|\mathbf{u}-\mathbf{u}^*\|\|_2/\#\mathcal{G}_0$	time
17^3	$1/16$	8	$2.110010 \cdot 10^{-2}$	$2.162535 \cdot 10^{-5}$	1.66 s
33^3	$1/32$	11	$5.078421 \cdot 10^{-3}$	$1.810825 \cdot 10^{-6}$	12.84 s
65^3	$1/64$	14	$1.251313 \cdot 10^{-3}$	$1.580911 \cdot 10^{-7}$	104.61 s
129^3	$1/128$	17	$3.112553 \cdot 10^{-4}$	$1.392736 \cdot 10^{-8}$	909.64 s

TABLE 4.2
Timings and error norms for a 33^3-problem with $h = 1/32$ and various refinements. The error of the method is only marginally affected by the number of refinement steps.

#refinements	$\#\mathcal{G}_{l_{\max}}$	$\|\|\mathbf{u}-\mathbf{u}^*\|\|_\infty$	$\|\|\mathbf{u}-\mathbf{u}^*\|\|_2/\#\mathcal{G}_0$
2	65^3	$5.089194 \cdot 10^{-3}$	$2.023222 \cdot 10^{-6}$
3	65^3	$5.085428 \cdot 10^{-3}$	$1.857736 \cdot 10^{-6}$
4	37^3	$5.066483 \cdot 10^{-3}$	$1.927579 \cdot 10^{-6}$
5	33^3	$5.063288 \cdot 10^{-3}$	$1.840964 \cdot 10^{-6}$
6	33^3	$5.079554 \cdot 10^{-3}$	$1.815541 \cdot 10^{-6}$
7	21^3	$5.067220 \cdot 10^{-3}$	$1.815151 \cdot 10^{-6}$
8	17^3	$5.070326 \cdot 10^{-3}$	$1.811852 \cdot 10^{-6}$
9	17^3	$5.084148 \cdot 10^{-3}$	$1.812722 \cdot 10^{-6}$
10	13^3	$5.084021 \cdot 10^{-3}$	$1.812488 \cdot 10^{-6}$
11	9^3	$5.078421 \cdot 10^{-3}$	$1.810825 \cdot 10^{-6}$
12	9^3	$5.084541 \cdot 10^{-3}$	$1.812455 \cdot 10^{-6}$
13	9^3	$5.088087 \cdot 10^{-3}$	$1.813763 \cdot 10^{-6}$
14	9^3	$5.089895 \cdot 10^{-3}$	$1.814523 \cdot 10^{-6}$
15	9^3	$5.090805 \cdot 10^{-3}$	$1.814928 \cdot 10^{-6}$
16	9^3	$5.091260 \cdot 10^{-3}$	$1.815137 \cdot 10^{-6}$
17	9^3	$5.091489 \cdot 10^{-3}$	$1.815244 \cdot 10^{-6}$
18	9^3	$5.091603 \cdot 10^{-3}$	$1.815297 \cdot 10^{-6}$
19	9^3	$5.091660 \cdot 10^{-3}$	$1.815324 \cdot 10^{-6}$
20	9^3	$5.091688 \cdot 10^{-3}$	$1.815337 \cdot 10^{-6}$

We ran the same test using the original method presented in [9], thus not setting the boundary values to the values of the continuous problem. We used FAC instead of MLAT for solving the linear system. The results in Table 4.3 and Fig. 4.2 show that this method behaves as expected: Increasing the number of grid refinements increases the accuracy of the method up to the same level than our modification.

Further we tested our modified method in a particle simulation code. Therefore the total electrostatic energy of a DNA fragment including counter ions consisting of 1316 atoms was calculated using different mesh sizes. Similarly to the example above, the point charges were replaced by cubic B-spline charge densities. This has been corrected afterwards by a near field correction. The results of this tests can be found in Table 4.4. One clearly sees, that the relative error of the energy is divided by four as the grid size is doubled, as expected.

5. Conclusion. We have presented a method that uses hierarchically coarsened and extended grids in order to compute the solution of the Poisson equation in free space. The method is similar to the method proposed by Washio and Oosterlee in [9], but the refinement process is stopped at some level and the Dirichlet boundary conditions derived from the con-

TABLE 4.3
Timings and error norms for a 33^3-problem with $h = 1/32$ and various refinements using the method of Washio and Oosterlee. The error of the method heavily depends on number of refinement steps, reaching the same accuracy as the modified method.

#refinements	$\#\mathcal{G}_{l_{\max}}$	$\|\|\mathbf{u}-\mathbf{u}^*\|\|_\infty$	$\|\|\mathbf{u}-\mathbf{u}^*\|\|_2/\#\mathcal{G}_0$
2	65^3	$3.653597 \cdot 10^{-2}$	$1.915066 \cdot 10^{-4}$
3	65^3	$1.783026 \cdot 10^{-2}$	$9.573523 \cdot 10^{-5}$
4	37^3	$1.584892 \cdot 10^{-2}$	$8.508257 \cdot 10^{-5}$
5	33^3	$8.995442 \cdot 10^{-3}$	$4.779984 \cdot 10^{-5}$
6	33^3	$4.631318 \cdot 10^{-3}$	$2.383245 \cdot 10^{-5}$
7	21^3	$3.762046 \cdot 10^{-3}$	$1.905511 \cdot 10^{-5}$
8	17^3	$2.929352 \cdot 10^{-3}$	$1.192743 \cdot 10^{-5}$
9	17^3	$4.014153 \cdot 10^{-3}$	$6.073405 \cdot 10^{-6}$
10	13^3	$4.375166 \cdot 10^{-3}$	$4.211756 \cdot 10^{-6}$
11	9^3	$4.554064 \cdot 10^{-3}$	$3.346295 \cdot 10^{-6}$
12	9^3	$4.821822 \cdot 10^{-3}$	$2.248768 \cdot 10^{-6}$
13	9^3	$4.956727 \cdot 10^{-3}$	$1.902828 \cdot 10^{-6}$
14	9^3	$5.024221 \cdot 10^{-3}$	$1.821841 \cdot 10^{-6}$
15	9^3	$5.057969 \cdot 10^{-3}$	$1.809017 \cdot 10^{-6}$
16	9^3	$5.074843 \cdot 10^{-3}$	$1.809788 \cdot 10^{-6}$
17	9^3	$5.083280 \cdot 10^{-3}$	$1.811972 \cdot 10^{-6}$
18	9^3	$5.087498 \cdot 10^{-3}$	$1.813512 \cdot 10^{-6}$
19	9^3	$5.089608 \cdot 10^{-3}$	$1.814394 \cdot 10^{-6}$
20	9^3	$5.090662 \cdot 10^{-3}$	$1.814863 \cdot 10^{-6}$

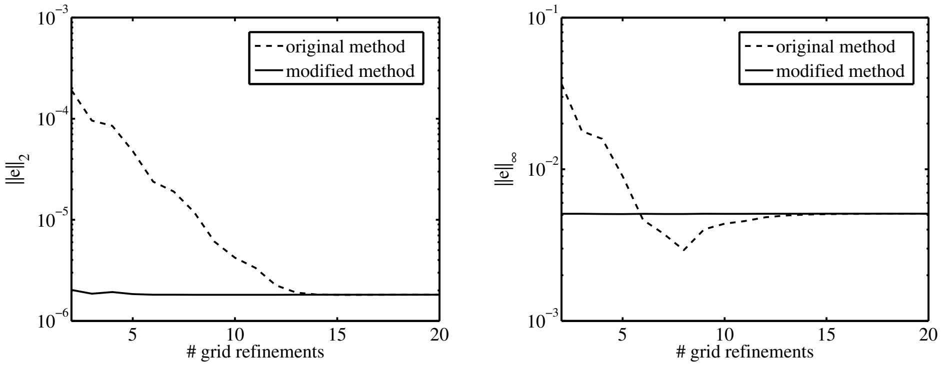

FIG. 4.2. *Behavior of the error of the original method and of our modification. Using the original method both, the error in the 2-norm and in the ∞-norm, depend heavily on the number of grid refinements. The accuracy converges to the accuracy of our modification, that is almost independent of the number of refinements.*

TABLE 4.4
Relative error of the total electrostatic energy of a 1316 atom DNA fragment calculated using a particle simulation code with the help of our modified method.

$\#\mathcal{G}_0$	h	$\|E-E^*\|/\|E^*\|$
17^3	$1/16$	$8.737377 \cdot 10^{-4}$
33^3	$1/32$	$2.303279 \cdot 10^{-4}$
65^3	$1/64$	$5.736910 \cdot 10^{-5}$
129^3	$1/128$	$1.287933 \cdot 10^{-5}$

tinous problem are imposed on that level. This is a major difference to their method, which in principle refines the grid infinitely many times.

We extended Washio's and Oosterlee's error analysis and we have shown that the introduction of the boundary conditions at the coarsest level does not influence the order of the method's accuracy. Therefore the modification enables the use of hierarchical grid coarsening without altering the accuracy by choosing a different number of refinement steps at very small costs.

We implemented the modified method. The numerical experiments show that the error behaves as expected and that the stopping at arbitrary levels does indeed not significantly influence the behaviour of the computed solution. Thus, the proposed method is suitable to compute the solution of Poisson's equation in free space using a multigrid method.

In the future, we plan to further optimize our implementation and to add higher-order conservative discretization schemes to both our analysis and our implementation. Additionally, we will work on the parallelization of our method, so that we can use it in large scale molecular dynamics simulations.

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