

On the Extension of Goal-Oriented Error Estimation and Hierarchical Modeling to Discrete Lattice Models

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Abstract

The Goals algorithm for adaptive modeling is extended to the case of discrete models such as those characterized by lattice structures (or the static behavior molecular systems) by using surrogate models obtained from continuum approximations of the lattice. The result is a technique that could provide for scale-bridging between continuum models and atomistic models, although the present development concerns only simple algebraic systems. An example is provided in which quantities of interest in a large number of degrees of freedom system are computed to a preset tolerance in relatively few low-order approximations.

Keywords: multiscale models, adaptive modeling, error estimates, continuum/lattice models.

1 Introduction

In earlier work [6, 8, 4], we developed techniques for assessing model and approximation error in solid and continuum mechanics, and methods for adapting the mathematical models of certain events to control modeling error. These techniques fall under the general heading of *hierarchical modeling* and *Goal-oriented a posteriori error estimation and model adaptivity*. A general theory for estimating modeling error was given in [4]. In the present paper, we extend this approach to the equilibrium analysis of “atomic” lattices, where the base model is defined by a regular periodic lattice and the surrogate models are obtained from continuum models characterized by PDE’s; precisely the opposite situation is encountered in modeling micro-scale effects in multi-phase heterogeneous materials [6, 8]. An important byproduct of our analysis is a new approach to modeling the transition from continuum models to “molecular” models. In particular, we present techniques in which the notion of convergence of finite element models of the continuum is unambiguously preserved, and in which convergence of the base molecular or lattice model is trivial. Thus, the notion of a continuum atomistic interface and coupling is precisely determined in a rigorous way.

The paper is organized as follows: In Section 2, we provide a brief summary of the procedure proposed in [4] to estimate the modeling errors with respect to some quantity of interest. We present in Section 3 a model problem for static equilibrium of a material lattice and introduce in Section 4 a simple problem which will be later referred to as the continuum model. The

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continuum model is given in terms of a partial differential equation and will be considered here as a surrogate problem of the lattice model problem. We apply in Section 5 the technique described in Section 2 to the continuum/lattice problems for estimating modeling errors, i.e. the difference between the solutions of the continuum and lattice models, and describe an adaptive algorithm for controlling modeling errors. We demonstrate in Section 6 the efficiency of the adaptive algorithm on two numerical examples. Conclusions are given in Section 7.

2 Modeling Errors in Quantities of Interest

The abstract setting for the theory of Goal-oriented estimation of modeling error is this: we wish to find a vector $\mathbf{u}$ in a topological vector space V such that

$$B(\mathbf{u}, \mathbf{v}) = F(\mathbf{v}) \quad \forall \mathbf{v} \in V \quad (1)$$

where $B(\cdot, \cdot)$ is a bilinear (or semilinear) form on V and F is a linear functional on V . Of interest is a quantity of interest $Q(\mathbf{u})$, Q being a functional on V . To characterize Q , we seek an influence vector $\mathbf{p}$ which is a solution of the dual problem,

$$B(\mathbf{v}, \mathbf{p}) = Q(\mathbf{v}) \quad \forall \mathbf{v} \in V \quad (2)$$

Problem (1) is called the primal base problem; problem (2) the dual base problem. If $B(\cdot, \cdot)$ is nonlinear in $\mathbf{u}$, we replace (2) by $B'(\mathbf{u}; \mathbf{v}, \mathbf{p}) = Q'(\mathbf{u}; \mathbf{v})$, where $B'(\cdot; \cdot, \cdot)$ and $Q'(\cdot; \cdot)$ are functional (Gâteaux) derivatives of $B(\cdot, \cdot)$ and $Q(\cdot)$ respectively.

The basic idea is that (1) and (2) are intractable: too complex or too large to be solved by any practical means. Therefore, we seek simpler *surrogate* problems that are tractable and of the form

$$\begin{aligned} B_0(\mathbf{u}_0, \mathbf{v}) &= F(\mathbf{v}) \quad \forall \mathbf{v} \in V \\ B_0(\mathbf{v}, \mathbf{p}_0) &= Q(\mathbf{v}) \quad \forall \mathbf{v} \in V \end{aligned} \quad (3)$$

$B_0(\cdot, \cdot)$ being a new bilinear form. In [4] (see also [2], it is shown that

$$Q(\mathbf{u}) - Q(\mathbf{u}_0) = R(\mathbf{u}_0, \mathbf{p}) \quad (4)$$

where $R(\mathbf{u}_0, \mathbf{v})$ is the residual functional

$$R(\mathbf{u}_0, \mathbf{v}) = F(\mathbf{v}) - B(\mathbf{u}_0, \mathbf{v}) \quad (5)$$

If the problem is nonlinear, the right-hand-side of (4) is replaced by $R(\mathbf{u}_0, \mathbf{p}) + r$, where r is a functional involving quadratic and higher terms in the errors $\mathbf{e}_0 = \mathbf{u} - \mathbf{u}_0$ and $\boldsymbol{\varepsilon}_0 = \mathbf{p} - \mathbf{p}_0$. In applications, we often neglect such higher order terms, and use $R(\mathbf{u}_0, \mathbf{p})$ as an approximation of $Q(\mathbf{u}) - Q(\mathbf{u}_0)$. The use of such relations to develop adaptive modeling schemes for estimating and controlling errors in modeling heterogeneous materials is described in [6, 8]. Our aim is to use (4) as a basis for estimating and controlling errors in models involving a combination of discrete and continuum attributes. Here, the base model is one provided by the discrete lattice structure, representing, for instance, a molecular dynamics system in equilibrium, and in which the surrogate model is to be constructed from a continuum model of the material.

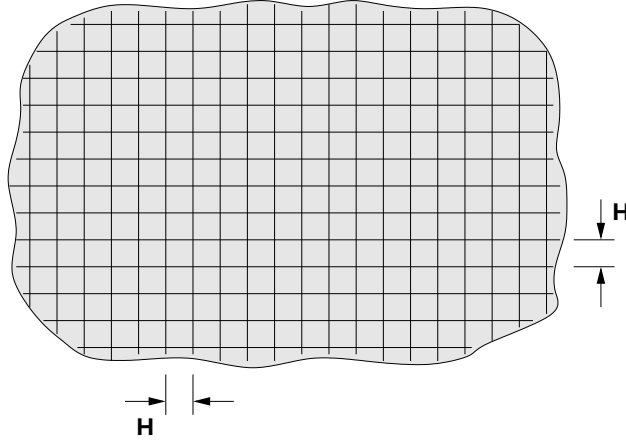


Figure 1: A regular periodic lattice in $\mathbb{R}^2$.

3 A Model Lattice Problem

To fix ideas, we consider a simple case of static equilibrium of a material lattice with regular periodic micro-structure. The regular lattice L has lattice uniform width H and extends indefinitely in $\mathbb{R}^d$, $d = 2$ or 3 . For the sake of simplicity, we only consider two-dimensional domains here, i.e. $d = 2$, as indicated in Fig. 1. All results presented in this report are easily extended to three-dimensional problems. The goal is to determine a discrete scalar field u which takes on values $u_{i,j}$ at each lattice point $\mathbf{x}_{i,j}$, $(i, j) \in \mathbb{Z}^2$, and which satisfies the equilibrium equation

$$\sum_{(i,j) \in \mathbb{Z}^2} a_{i,j} u_{i,j} - f_{i,j} = 0 \quad (6)$$

where $f_{i,j} = f(\mathbf{x}_{i,j})$, f being an (i, j) -periodic prescribed force field, and $a_{i,j}$ are appropriate constants.

To further restrict the problem while also establishing conditions sufficient to guarantee the existence of solutions to (1), we shall make the following simplifications:

1. A subdomain $\Omega = (0, a) \times (0, b) \subset \mathbb{R}^2$ is identified with origin $(0, 0)$ at a lattice point, as shown in Fig. 2, and the lengths a and b are naturally chosen as multiples of H . Note that in more general settings, Ω can be a more complex domain than just a rectangle and may depend on the structure of the lattice as well.
2. The boundary of Ω is denoted $\partial\Omega$ and $u_{i,j} = 0$ at points $\mathbf{x}_{i,j} \in \partial\Omega$.
3. $f_{i,j}$ is given at all points $\mathbf{x}_{i,j} \in \overline{\Omega}$.
4. The coefficients representing the interactions of adjacent "atoms" at sites in the lattice are given.

For simplicity, one example is the difference stencil,

$$-\frac{1}{H^2}u_{i-1,j} - \frac{1}{H^2}u_{i,j-1} + \frac{4}{H^2}u_{i,j} - \frac{1}{H^2}u_{i+1,j} - \frac{1}{H^2}u_{i,j+1} - f_{i,j} = 0 \quad (7)$$

which we write in matrix form as

$$\mathbf{A}\mathbf{u} = \mathbf{f} \quad (8)$$

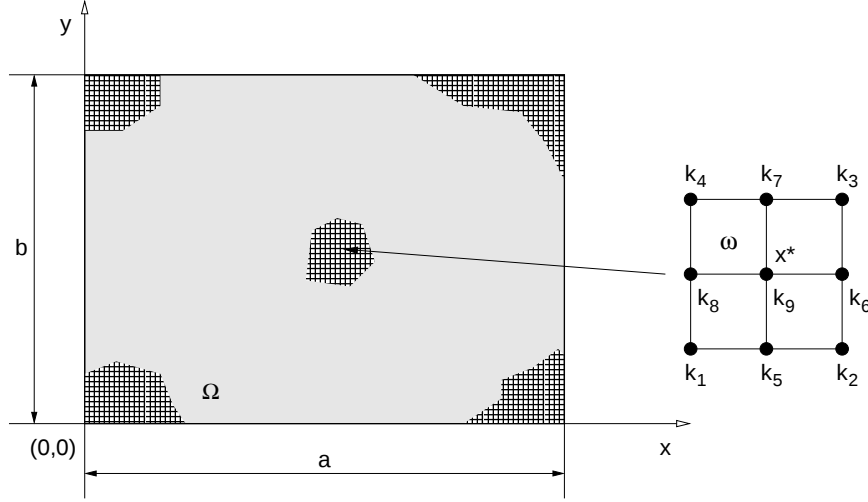


Figure 2: A subdomain Ω of $\mathbb{R}^2$ and an interior patch ω of four cells surrounding lattice site $\mathbf{x}^* = (x^*, y^*)$.

where $\mathbf{u}$ and $\mathbf{f}$ are N -vectors and $\mathbf{A}$ is an $N \times N$ matrix, assuming there are N lattice points in the closure of Ω .

In a more abstract setting, we introduce the finite dimensional vector space

$$V_L = \{\mathbf{v} \in \mathbb{R}^N, v_k = \text{component of } \mathbf{v} \text{ corresponding to lattice point } \mathbf{x}_k \in \overline{\Omega}, v_k = 0 \text{ on } \partial\Omega\} \quad (9)$$

and the bilinear and linear forms,

$$\begin{aligned} B : V_L \times V_L &\rightarrow \mathbb{R}; & B(\mathbf{u}, \mathbf{v}) &= \mathbf{v}^T \mathbf{A} \mathbf{u} \\ F : V_L &\rightarrow \mathbb{R}; & F(\mathbf{v}) &= \mathbf{v}^T \mathbf{f} \end{aligned} \quad (10)$$

Then, the lattice equilibrium problem is

$$\text{Find } \mathbf{u} \in V_L \text{ such that } B(\mathbf{u}, \mathbf{v}) = F(\mathbf{v}) \quad \forall \mathbf{v} \in V_L \quad (11)$$

Our goal is not to calculate $\mathbf{u}$, but some functional of $\mathbf{u}$ defined by a *quantity of interest* $Q(\mathbf{u})$. For example, if ω is a patch of four cells surrounding a particular lattice point $\mathbf{x}^*$ (see Fig. 2), we may be interested in the weighted average value of $\mathbf{u}$ over the cell:

$$\begin{aligned} Q(\mathbf{u}) &= \frac{1}{16} \left[(u_{k_1} + u_{k_2} + u_{k_3} + u_{k_4}) + 2(u_{k_5} + u_{k_6} + u_{k_7} + u_{k_8}) + 4u_{k_9} \right] \\ &= \sum_{l=1}^9 w_{k_l} u_{k_l} \end{aligned} \quad (12)$$

w_{k_l} being the indicated weights. This corresponds to the average of the interpolant of u over the patch ω . The problem of finding a vector $\mathbf{p} \in V_L$ such that

$$B(\mathbf{v}, \mathbf{p}) = Q(\mathbf{v}) \quad \forall \mathbf{v} \in V_L \quad (13)$$

is then the *base dual problem* for the functional Q , and $\mathbf{p}$ is the *dual solution* or *influence vector* for the lattice problem.

4 A Continuum Surrogate Problem

We propose here a simple continuum model deduced from the lattice model. Our principal motivation in this paper is to focus on the adaptive algorithm rather than modeling issues. Various techniques have been suggested to derive continuum models, see for example [3, 7]. For the lattice model (8), in the limit as $H \rightarrow 0$, we consider here the following continuum model of the problem:

$$\text{Find } u_0 \in V \text{ such that } B_0(u_0, v) = F_0(v) \quad \forall v \in V \quad (14)$$

and

$$\text{Find } p_0 \in V \text{ such that } B_0(v, p_0) = Q_0(v) \quad \forall v \in V \quad (15)$$

where now

$$B_0(u, v) = \int_{\Omega} \nabla u \cdot \nabla v \, dx dy \quad (16)$$

$$F_0(v) = \int_{\Omega} f v \, dx dy \quad (17)$$

$$Q_0(v) = \frac{1}{|\omega|} \int_{\omega} v \, dx dy \quad (18)$$

$$V = \{v \in H^1(\Omega) : v = 0 \text{ on } \partial\Omega\} = H_0^1(\Omega) \quad (19)$$

Clearly, in the limit as $H \rightarrow 0$, the lattice model (8) converges to the model of the Poisson problem $-\Delta u = f$ in Ω , $u = 0$ on $\partial\Omega$. Of course, the spaces V_L and V are now incompatible, V_L being of dimension N and V infinite dimensional.

We must next map the continuum description onto the lattice model to be able to compare errors in the quantities of interest. This is done as follows. Let $\Pi : V \rightarrow V_L$ denote a (collocation) mapping from V onto V_L defined by

$$\begin{aligned} \Pi w &= \mathbf{v} = \{v_k\}_{k=1}^N \\ v_k &= w_{\rho}(\mathbf{x}_k) = \int_{B_{\rho}(\mathbf{x}_k)} k_{\rho}(\mathbf{x}, \mathbf{x}_k) w(\mathbf{x}) \, dx \\ \rho &\ll H \\ \mathbf{x}_k &= \text{lattice site in } L \end{aligned} \quad (20)$$

Here $B_{\rho}(\mathbf{x}_k)$ is a ball of radius ρ centered at the lattice node $\mathbf{x}_k$, $k_{\rho}(\mathbf{x}, \mathbf{x}_k)$ is a smooth kernel vanishing outside $B_{\rho}(\mathbf{x}_k)$ and normalized so that

$$\int_{B_{\rho}(\mathbf{x}_k)} k_{\rho}(\mathbf{x}, \mathbf{x}_k) \, dx = 1.$$

Thus, w_{ρ} is the mollifier (or mollification) of w . The operator Π thus produces an N -vector in V_L defined on the lattice whose components are simply the values of the functions w in V , smoothed so that their pointwise values are well-defined (the functions $w \in V$, being in $H^1(\Omega)$, are not necessarily continuous for 2D and 3D domains). In practice, we replace w_{ρ} by finite element approximations w_h for mesh size h sufficiently small. This is discussed in Section 5, to follow.

Applying the ideas of Section 2, we now derive an estimate for the modeling error. Let $u_0 \in V$ be the unique solution of (14) and $\mathbf{p} \in V_L$ be the influence vector for Q satisfying

(13). Then, according to (4), the modeling error $\mathbf{e}_0 = \mathbf{u} - \Pi u_0 = \mathbf{u} - \mathbf{u}_0$ in the quantity of interest Q is

$$Q(\mathbf{e}_0) = Q(\mathbf{u}) - Q(\mathbf{u}_0) = R(\mathbf{u}_0, \mathbf{p}). \quad (21)$$

We can rewrite the residual as:

$$R(\mathbf{u}_0, \mathbf{p}) = R(\mathbf{u}_0, \mathbf{p}_0) + R(\mathbf{u}_0, \boldsymbol{\varepsilon}_0) \quad (22)$$

$$= R(\mathbf{u}_0, \mathbf{p}_0) + B(\mathbf{e}_0, \boldsymbol{\varepsilon}_0) \quad (23)$$

where $\mathbf{p}_0 = \Pi p_0$, p_0 being the influence function for the surrogate problem (15), and $\boldsymbol{\varepsilon}_0 = \mathbf{p} - \mathbf{p}_0$. Note that (23) follows from (22) by making use of the error equation $B(\mathbf{e}_0, \mathbf{v}) = R(\mathbf{u}_0, \mathbf{v})$, $\forall \mathbf{v} \in V$ and by taking $\mathbf{v} = \boldsymbol{\varepsilon}_0$. An estimate of the modeling error is then obtained by neglecting the higher order term $B(\mathbf{e}_0, \boldsymbol{\varepsilon}_0)$ so that $Q(\mathbf{e}_0) \approx R(\mathbf{u}_0, \mathbf{p}_0)$, or by computing bounds on $B(\mathbf{e}_0, \boldsymbol{\varepsilon}_0)$ as in [6], or computing the exact dual solution vector $\mathbf{p}$.

5 Approximations of the Continuum Model

5.1 Discrete approximations

In general, the continuum models (14) and (15) cannot be solved exactly, and numerical approximations, such as finite element approximations, of u_0 and p_0 , must be obtained. Then, instead of (20), a more direct construction of a mapping from V onto V_L can be defined.

Let $\{P_h\}$ denote a family of partitions of Ω into finite elements K each being the image under invertible maps F_K of a master element $\hat{K}$ over which polynomial test functions are defined (see, e.g. [1]). We shall assume that the partitions are *regular* and that the usual interpolation properties of finite element interpolation of functions in Sobolev spaces are in force [5]. In this way, we generate a *family* of finite-dimensional subspaces $\{V^h\}$ of V , with $\bigcup_{h>0} V^h$ everywhere dense in, say, $H^1(\Omega)$. For a given subspace V^h , the finite element approximations of (14) and (15) are thus

$$B_0(u_0^h, v^h) = F_0(v^h) \quad \forall v^h \in V^h \quad (24)$$

$$B_0(v^h, p_0^h) = Q_0(v^h) \quad \forall v^h \in V^h \quad (25)$$

Instead of (20), we introduce the “collocation” operator $\Pi^h: V^h \rightarrow V_L$ such that

$$\begin{aligned} \Pi^h v^h &= \mathbf{v}^h = \{(v^h)_k\}_{k=1}^N \\ (v^h)_k &= v^h(\mathbf{x}_k) \\ \mathbf{x}_k &= \text{lattice site in } \overline{\Omega} \end{aligned} \quad (26)$$

5.2 Estimate of modeling error

To estimate the error in $Q(\mathbf{u}_0^h)$, we proceed as before. Using $\mathbf{u}_0^h = \Pi^h u_0^h$ and $\mathbf{p}_0^h = \Pi^h p_0^h$ instead of $\mathbf{u}_0$ and $\mathbf{p}_0$, respectively, the estimate (21) becomes

$$\begin{aligned} Q(\mathbf{u}) - Q(\mathbf{u}_0^h) &= R(\mathbf{u}_0^h, \mathbf{p}) \\ &= R(\mathbf{u}_0^h, \mathbf{p}_0^h) + B(\mathbf{u} - \mathbf{u}_0^h, \mathbf{p} - \mathbf{p}_0^h) \end{aligned} \quad (27)$$

Neglecting the higher order term in $\mathbf{u} - \mathbf{u}_0^h$, we then obtain the error estimate:

$$\mathcal{E} = R(\mathbf{u}_0^h, \mathbf{p}_0^h) \approx Q(\mathbf{u}) - Q(\mathbf{u}_0^h) \quad (28)$$

It is important to note that there is no connection between the lattice dimension H and the mesh size h . Convergence of the finite element approximation is unambiguous: as $h \rightarrow 0, u_0^h \rightarrow u_0$ in $H^1(\Omega)$, independently of H (for quasi-uniform refinements, with $h = \max h_K, h_K = \text{dia}(K)$).

5.3 Adaptive modeling strategy

We now describe an adaptive modeling strategy aimed at reducing computational costs. For instance, let us suppose that we cannot solve the N -order system (11), N being a large number, but that we wish to compute for the vector $\mathbf{u}$ the quantity of interest $Q(\mathbf{u})$ to within a tolerance γ_{tol} , i.e.

$$\frac{|Q(\mathbf{u}) - Q(\mathbf{u}_0^h)|}{|Q(\mathbf{u})|} \leq \gamma_{tol}.$$

We propose a Goal-oriented hierarchical modeling algorithm that employs concepts similar to those developed in [6, 8] for computing local features in a lattice. Again, let L denote the lattice of N sites covering the domain Ω with lattice width H . In addition, let Ω be partitioned into K cells of size larger than H (see Fig. 3). The error estimate $\mathcal{E}$ can then be decomposed into contributions over each cell as

$$\mathcal{E} = \mathcal{R}(\mathbf{u}_0^h, \mathbf{p}_0^h) = \sum_{n=1}^K \mathcal{R}_n(\mathbf{u}_0^h, \mathbf{p}_0^h) \quad (29)$$

where $\mathcal{R}_n(\mathbf{u}_0^h, \mathbf{p}_0^h)$ denotes the contribution in the n^{th} cell to the total error $\mathcal{E}$. More explicitly, recall that

$$\begin{aligned} \mathcal{R}(\mathbf{u}_0^h, \mathbf{p}_0^h) &= F(\mathbf{p}_0^h) - B(\mathbf{u}_0^h, \mathbf{p}_0^h) \\ &= \mathbf{p}_0^{hT} \mathbf{f} - \mathbf{p}_0^{hT} A \mathbf{u}_0^h \\ &= \mathbf{p}_0^{hT} (\mathbf{f} - A \mathbf{u}_0^h) \\ &= \sum_{k=1}^N \mathbf{p}_{0k}^h \left(\mathbf{f}_k - \sum_{l=1}^N A_{kl} \mathbf{u}_{0l}^h \right) \end{aligned}$$

Then the contribution $\mathcal{E}_n$ from the n^{th} cell Θ_n is computed according to

$$\mathcal{E}_n = \mathcal{R}_n(\mathbf{u}_0^h, \mathbf{p}_0^h) = \sum_{k=1}^N \beta_k^n \left[\mathbf{p}_{0k}^h \left(\mathbf{f}_k - \sum_{l=1}^N A_{kl} \mathbf{u}_{0l}^h \right) \right] \quad (30)$$

where the coefficients β_k^n depend on the location of the sites $\mathbf{x}_k$ with respect to the cell Θ_n . Let θ_k be the number of cells that contain point $\mathbf{x}_k$. This number can take on the values 4, 2, or 1, depending on whether $\mathbf{x}_k$ is an interior site of L , or lies on one of the boundary edges of L , or is one of the four corners of L , respectively. Then

$$\beta_k^n = \begin{cases} 0 & \text{if } x_k \notin \bar{\Theta}_n \\ \theta_k^{-1} & \text{if } x_k \in \bar{\Theta}_n \end{cases}$$

The algorithm for adaptively modeling the lattice model with a continuum model is as follows:

1. Set $s = 0$
2. Replace the lattice model with the continuum model (14) and solve for a (very accurate) finite element approximation u_0^h of u_0 . Compute also an approximation p_0^h of p_0 .
3. Evaluate $\mathbf{u}_0^h = \Pi^h u_0^h$, $\mathbf{p}_0^h = \Pi^h p_0^h$, and the quantity of interest $Q(\mathbf{u}_0^h)$.
4. Estimate the error in $Q(\mathbf{u}_0^h)$ using (28), i.e. compute $\mathcal{E}^{(0)} = R(\mathbf{u}_0^h, \mathbf{p}_0^h)$.
5. Check whether $|\mathcal{E}^{(0)}|/|Q(\mathbf{u}_0^h) + \mathcal{E}^{(0)}| \leq \gamma_{tol}$? If yes, stop. If not, start the adaptive process.
6. Set $s = s + 1$
 - (a) Compute the cell contributions $\mathcal{E}_n = \mathcal{R}_n(\mathbf{u}_{s-1}^h, \mathbf{p}_{s-1}^h)$, $n = 1, \dots, K$ as in (30). Construct the patch L_s made of the cells that have not been already refined and that satisfy

$$\frac{|\mathcal{E}_n|}{\max_n |\mathcal{E}_n|} \geq \alpha$$

where α is a user-defined parameter.

- (b) Solve the reduced lattice problem on L_s for lattice vectors $\mathbf{u}_s^h$ and $\mathbf{p}_s^h$, with $\mathbf{u}_s^h = \mathbf{u}_0^h$ and $\mathbf{p}_s^h = \mathbf{p}_0^h$ at the points outside of L_s .
- (c) Estimate the error in $Q(\mathbf{u}_s^h)$, i.e. compute $\mathcal{E}^{(s)} = R(\mathbf{u}_s^h, \mathbf{p}_s^h)$.
- (d) Check whether $|\mathcal{E}^{(s)}|/|Q(\mathbf{u}_s^h) + \mathcal{E}^{(s)}| \leq \gamma_{tol}$? If the answer is negative, go to step 6. If the answer is affirmative, stop the adaptive process.

In this manner, we create a sequence of surrogate problems $\mathcal{P}_s$, whose solutions are given by $(\mathbf{u}_s^h, \mathbf{p}_s^h)$, $s = 0, 1, \dots$. The initial surrogate problem $\mathcal{P}_0$ is obtained using the continuum model only. The subsequent problems $\mathcal{P}_s$, $s = 1, 2, \dots$, combine the solutions from the continuum model and from the lattice model used only in the reduced lattice L_s . Obviously, this is only one example of many possible variants of the adaptive process. Note that the overall approach is also reminiscent of the multigrid method in which the lattice model stands for the the fine-scale grid, and the surrogate model for the coarse-scale grid model.

6 Numerical Examples

To demonstrate the Goals algorithm for adaptive modeling, we consider examples of regular lattices L on the square domain $\Omega = (0, 1)^2$ with lattice width $H = (m - 1)^{-1}$, $m = 11, 21, \dots, 61$. The lattice L is then made of $N = m^2$ sites such that:

$$L = \{(x_i, y_j) : i, j \in \mathbb{N}, 0 \leq i, j \leq m - 1, x_i = iH, y_j = jH\}$$

and will be referred to as a $m \times m$ lattice. We emphasize that the lattice solution is our solution of reference, although in these examples, the scales provided by the finite element solutions are finer. Again our only concern here is to demonstrate the feasibility of the adaptive strategy.

In all examples, we partition the domain Ω into 25 cells of dimension 0.2×0.2 (see Fig. 3) and the quantity of interest is the weighted average over the square domain ω of dimension $2H \times 2H$ located at the center of the lattice, as defined in (12). In other words, the

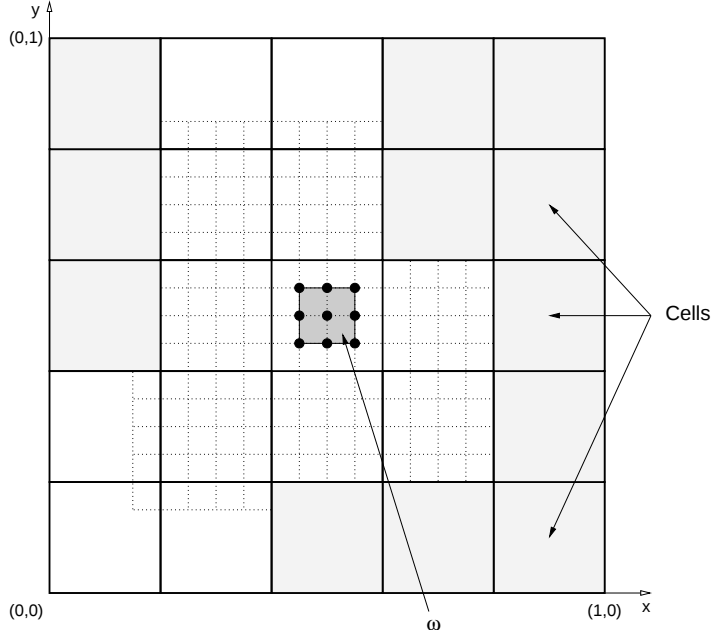


Figure 3: A lattice in $\mathbb{R}^2$.

quantity of interest is the weighted average of $\mathbf{u}$ at the lattice points $\mathbf{x}_{i,j}$ where $i, j \in \{(m-1)/2-1, (m-1)/2, (m-1)/2+1\}$. Note that the quantity of interest depends indirectly on the lattice width H .

The exact solution to the continuum model problem is given by

$$-\Delta u_0 = f, \quad \text{in } \Omega \quad u_0 = 0 \quad \text{on } \partial\Omega$$

where the datum f is determined such that $u_0(x, y)$ is known analytically. We will consider in the following two different functions u_0 . The solution of the Poisson problem is approximated using a mesh of 200×200 bilinear elements. In all numerical experiments, the parameter α introduced in step 6(a) of the adaptive algorithm will be chosen to be 0.5.

6.1 Example one

In this example, the continuum and lattice problems are set up in such a way that the exact continuum solution is given by

$$u_0(x, y) = 256x^2(1-x)^2y^2(1-y)^2e^{-100((x-0.25)^2+(y-0.25)^2)}$$

The function u_0 is essentially a differenced Gaussian centered at the point $(0.25, 0.25)$ as shown in Fig. 4. The term $x^2(1-x)^2y^2(1-y)^2$ ensures that u_0 and the derivatives of u_0 are zero on the boundary of Ω . The corresponding lattice solutions are shown in Fig. 5 for the 11×11 and 31×31 lattices. We show in Figs. 6 and 7 the continuum influence function p_0 and lattice influence influence $\mathbf{p}$ associated with the weighted average defined above, for the 11×11 and 31×31 lattices, respectively. As expected, we observe that the influence function becomes more localized as the lattice width decreases since, in all cases, the quantity of interest is defined with respect to the nine lattice points at the center of the lattice.

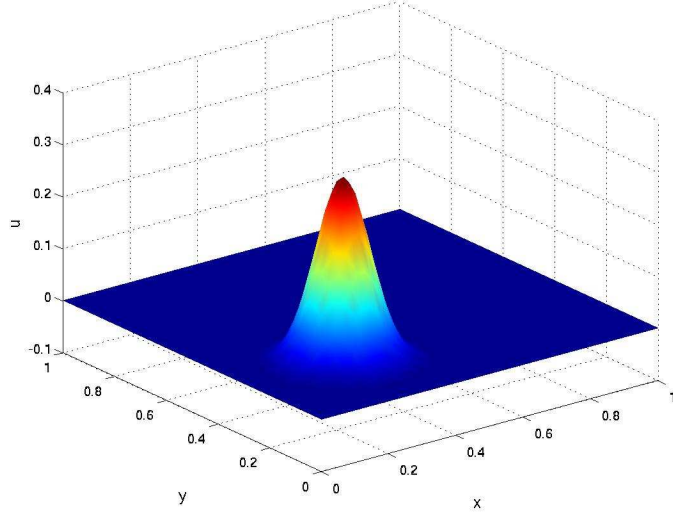


Figure 4: Accurate approximation of the continuum solution u_0 for example 1.

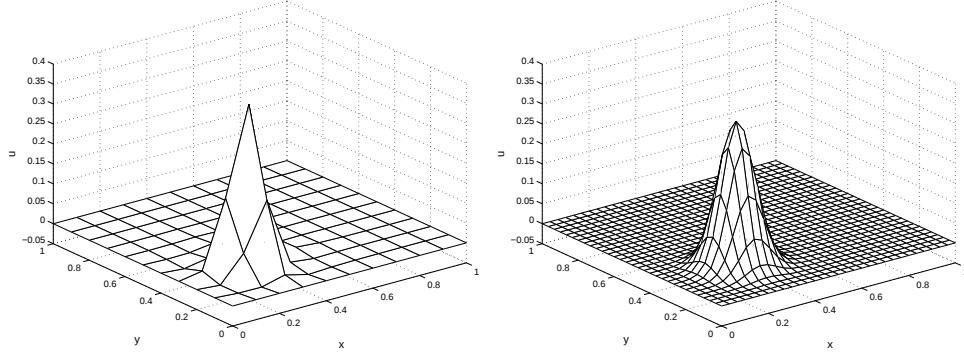


Figure 5: Lattice solutions of example 1 computed on the 11×11 and 31×31 lattices.

In the next set of numerical experiments, we test the adaptive modeling strategy proposed in Section 5.3. We set the tolerance on the error γ_{tol} to 5 percent. Figures 8 and 9 show the sequence of refinements for the 21×21 lattice. In these plots, and in all similar plots that follow, the grey area represents the subregion in which the solution has been computed using the continuum model, that is, u_0 . The complementary subregion displaying the lattice corresponds to the reduced lattice L_s , where s is the number of iterations already performed, as explained in Section 5.3. The number $l \leq s$ in the various cells indicates the iteration at which the cell has been added to the lattice L_s . In this case, eight refinements were necessary to achieve a tolerance of 5 percent which resulted in all but three cells being refined. Note that all plots are symmetric with respect to the diagonal $x = y$, as expected.

We show in Fig. 10 the final configurations obtained by adaptive modeling for all lattices. We observe that eight iterations are needed for the 11×11 and 21×21 lattices to achieve a tolerance of 5 percent on the error in the quantity of interest. For all the other lattices, the algorithm yields the same final configuration after 5 iterations, but note that the cells are

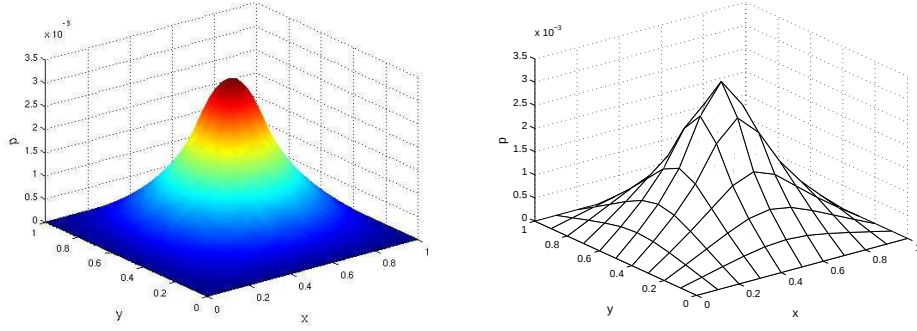


Figure 6: Influence functions associated with the 11×11 lattice: (left) continuum solution p_0 and (right) lattice solution $\mathbf{p}$.

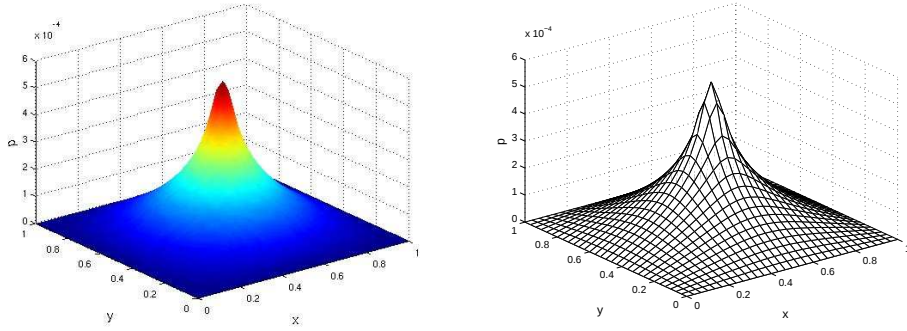


Figure 7: Influence functions associated with the 31×31 lattice: (left) continuum solution p_0 and (right) lattice solution $\mathbf{p}$.

not necessarily refined in the same order in all cases.

In Fig. 11, we show the effectivity indices and the evolution of the relative errors with respect to the number of refinements obtained by adaptive modeling. The effectivity indices provide a measure of the quality of the error estimates and are calculated as the ratio of the error estimate $\mathcal{E}^{(s)}$ at iteration s and the exact error, i.e.

$$\lambda = \frac{|\mathcal{E}^{(s)}|}{|Q(\mathbf{u}) - Q(\mathbf{u}_s^h)|}$$

Thus, an effectivity index of exactly one indicates that the error estimator perfectly estimates the exact error. From Fig. 11, we observe that the effectivity indices oscillates between 0.95 and 1.1 except for one value. The rates of convergence are mostly monotonic apart from the case of the 11×11 lattice. In this case, we believe that some internal boundary conditions obtained from the continuum solution are in error and greatly increase the relative error in the quantity of interest until these boundaries become part of the lattice by including the adjacent cells.

Finally, we show in Fig. 12, for illustration purposes, the solutions obtained on the reduced lattices L_3 (after the third iteration) for the 11×11 and 31×31 lattices. These plots can be qualitatively compared to the solutions that were computed on either the full continuum

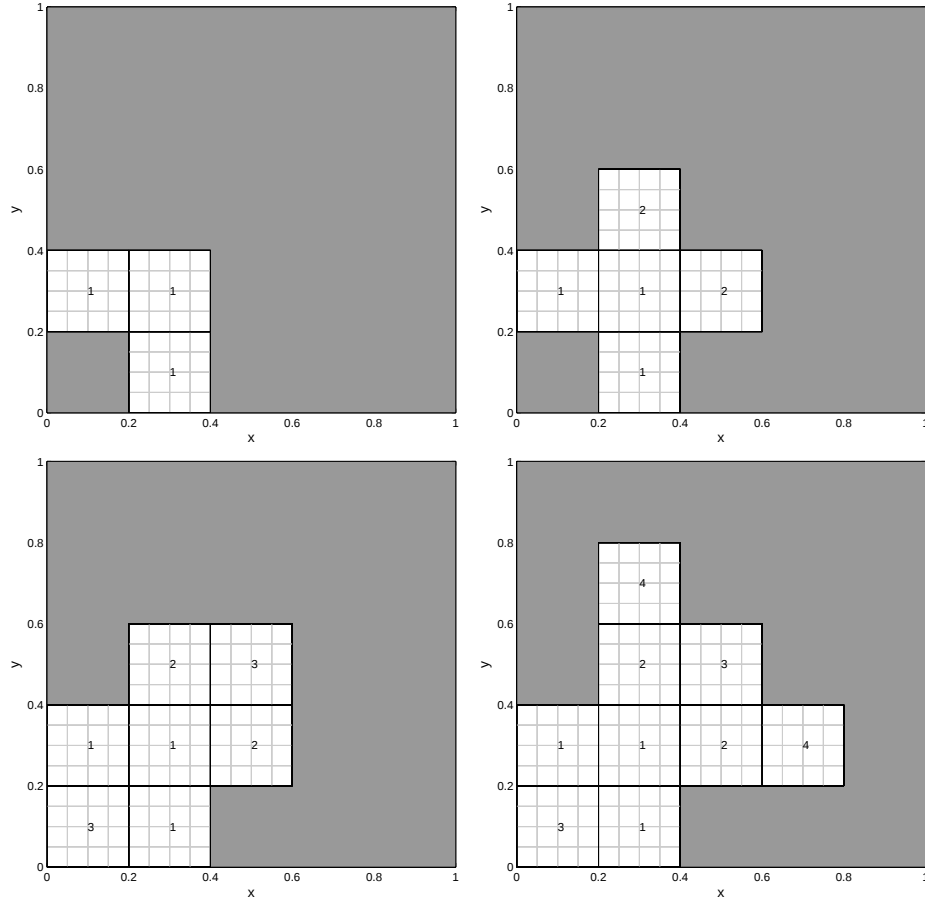


Figure 8: Sequence of surrogate models obtained by adaptive refinement for the 21×21 lattice (iterations $s = 1$ to 4). In these plots, the grey area represents the subregion in which the solution is obtained using the continuum model. The complementary subregion corresponds to the reduced lattice L_s . The number $l \leq s$ in the cells indicates the iteration at which the cell has been added to the lattice L_s .

model or the full lattice model; see Figs. 4 and 5.

6.2 Example two

We repeat in this section the same types of numerical experiments as before but for a different exact solution of the continuum model. Here the solution u_0 (see Fig. 13) is obtained by superposition of two “Gaussian functions” centered at the points $(0.25, 0.25)$ and $(0.50, 0.80)$ such that:

$$u_0(x, y) = 128x^2(1-x)^2y^2(1-y)^2e^{-100((x-0.25)^2+(y-0.25)^2)} + 512x^2(1-x)^2y^2(1-y)^2e^{-100((x-0.50)^2+(y-0.80)^2)}$$

In this case, the weighted average error, still computed over the nine points at the center of the lattices, is essentially influenced by the sources of error generated at the location of the

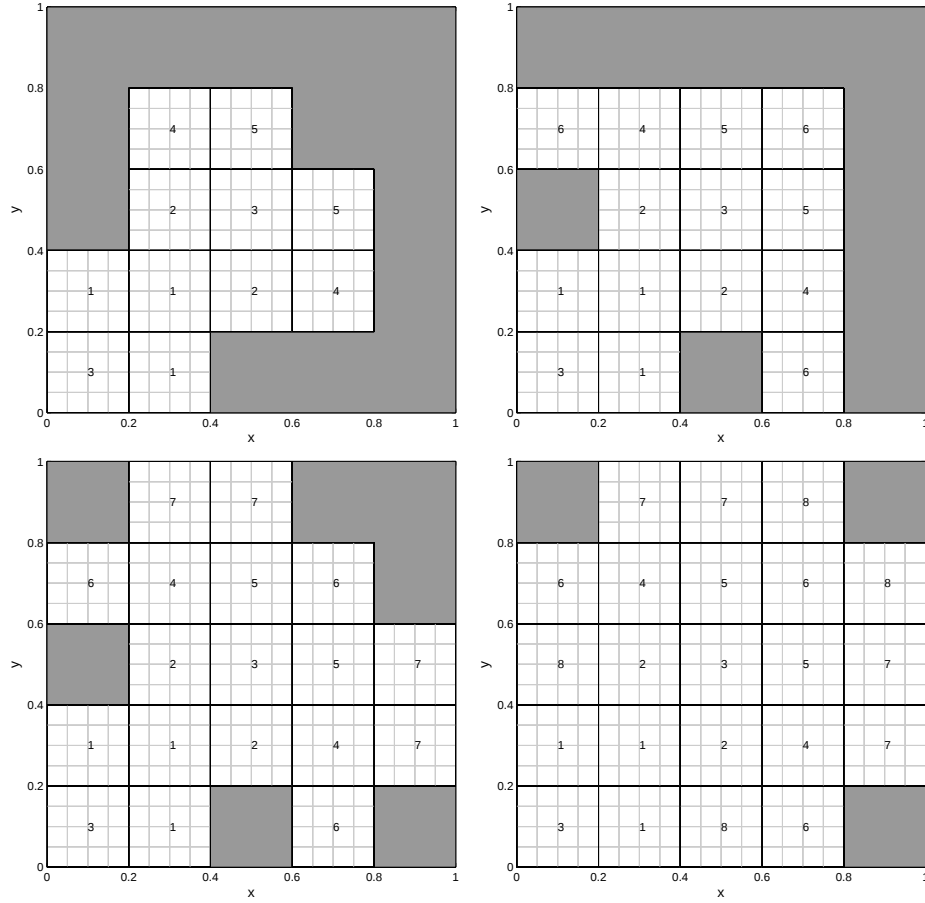


Figure 9: Sequence of surrogate models obtained by adaptive refinement for the 21×21 lattice (iterations $s = 5$ to 8). In these plots, the grey area represents the subregion in which the solution is obtained using the continuum model. The complementary subregion corresponds to the reduced lattice L_s . The number $l \leq s$ in the cells indicates the iteration at which the cell has been added to the lattice L_s .

two Gaussian functions. The corresponding lattice solutions are shown in Fig. 14 for the 11×11 and 31×31 lattices. Since the quantities of interest are the same as in example 1, so are the associated influence functions.

For testing the adaptive modeling strategy proposed in Section 5.3, we select two tolerances, i.e. $\gamma_{tol} = 10$ percent and $\gamma_{tol} = 5$ percent. Fig. 15 shows the sequence of refinements for the 21×21 lattice. The algorithm automatically performed five refinements in order to achieve a tolerance of 10 percent. We observe that the procedure essentially refines the cells that cover the peaks of the Gaussian functions and the features of the quantity of interest. The final configurations for all lattices are shown in Fig. 16 for $\gamma_{tol} = 10$ percent and in Fig. 17 for $\gamma_{tol} = 5$ percent. We observe that, apart from the 11×11 lattice, two to three extra iterations are necessary to reduce the error from 10 percent to 5 percent. The evolution of the effectivity indices and relative errors with respect to the number of refinements are displayed in Figs. 18 and 19. The convergence results suggest that the adaptive algorithm could be improved for our particular choice of quantity of interest. The erratic behavior prior

to a dramatic reduction in error may be attributed to the fact that the sequence of model enrichments employs local error measures rather than global error measures. Regardless of the rate of convergence, quite acceptable, indeed excellent, estimates of the modeling error are obtained. A more detailed study of various adaptive strategies and convergence will be undertaken for more complex systems in future studies. Finally the solutions obtained on the reduced lattices L_2 for the 11×11 and 31×31 lattices are given in Fig. 20 and should be compared with the solutions of Figs. 13 and 14. These pictures clearly demonstrate that the proposed adaptive procedure automatically refines the regions in which the large sources of modeling error contribute the most to the error in the quantity of interest.

7 Concluding Remarks

We have described in this paper a method to extend the Goals algorithm for adaptive modeling to the case of discrete models by using a continuum model for the surrogate problem. The method involves the derivation of a Goal-oriented error estimator to obtain computable error measures of local quantities of interest. The proposed adaptive algorithm is an iterative procedure which allows one to determine the regions of the domain in which it is necessary to use the lattice base model to control the error in the quantity of interest to within some preset tolerance. The solution of the continuum model is merely used to prescribe the internal boundary conditions for the reduced lattice problems. The methodology was tested here on two numerical examples and the results clearly demonstrate the great potential of this approach. In these examples, the continuum model is defined as a Poisson problem and the lattice model was derived by using a five-point central difference stencil for the Poisson equation. The main conclusion from this study is that it is actually feasible to automatically select the sites of the lattice that need be included in the reduced lattice problem to obtain accurate quantities of interest. Whenever the lattice problem is more expensive to solve than the continuum problem, the use of this approach would allow for substantial cost reductions. Our objective in the near future is to extend this methodology to molecular statics or molecular dynamics for problems in nanomechanics. The main issue will be to construct adequate surrogate problems from the lattice problems for multi-scale modeling and to deal with the loss of scale information due to the transition from the molecular model to the continuum model.

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References

- [1] M. AINSWORTH AND J. T. ODEN, *A Posteriori Error Estimation in Finite Element Analysis*, John Wiley & Sons, 2000.
- [2] M. BRAACK AND A. ERN, *A posteriori control of modeling errors and discretization errors*, Multiscale Model. Simul, 1 (2003), pp. 221–238.
- [3] P.-J. MARTINSSON AND G. J. RODIN, *Asymptotic expansions of lattice Green's functions*, Proc. R. Soc. Lond. A, 458 (2002), pp. 2609–2622.

- [4] J. T. ODEN AND S. PRUDHOMME, *Estimation of modeling error in computational mechanics*, Journal of Computational Physics, 182 (2002), pp. 496–515.
- [5] J. T. ODEN AND J. N. REDDY, *An Introduction to the Mathematical Theory of Finite Elements*, John Wiley & Sons, New-York, 1976.
- [6] J. T. ODEN AND K. VEMAGANTI, *Estimation of local modeling error and goal-oriented modeling of heterogeneous materials; Part I: error estimates and adaptive algorithms*, Journal of Computational Physics, 164 (2000), pp. 22–47.
- [7] V. B. SHENOY, R. MILLER, E. B. TADMOR, D. RODNEY, R. PHILLIPS, AND M. ORTIZ, *An adaptive finite element approach to atomic-scale mechanics—the quasicontinuum approach*, Journal of the Mechanics and Physics of Solids, 47 (1999), pp. 611–642.
- [8] K. VEMAGANTI AND J. T. ODEN, *Estimation of local modeling error and goal-oriented adaptive modeling of heterogeneous materials: II. a computational environment for adaptive modeling of heterogeneous elastic solids*, Comput. Meth. Appl. Mech. Engrg., 190 (2001), pp. 6089–6124.

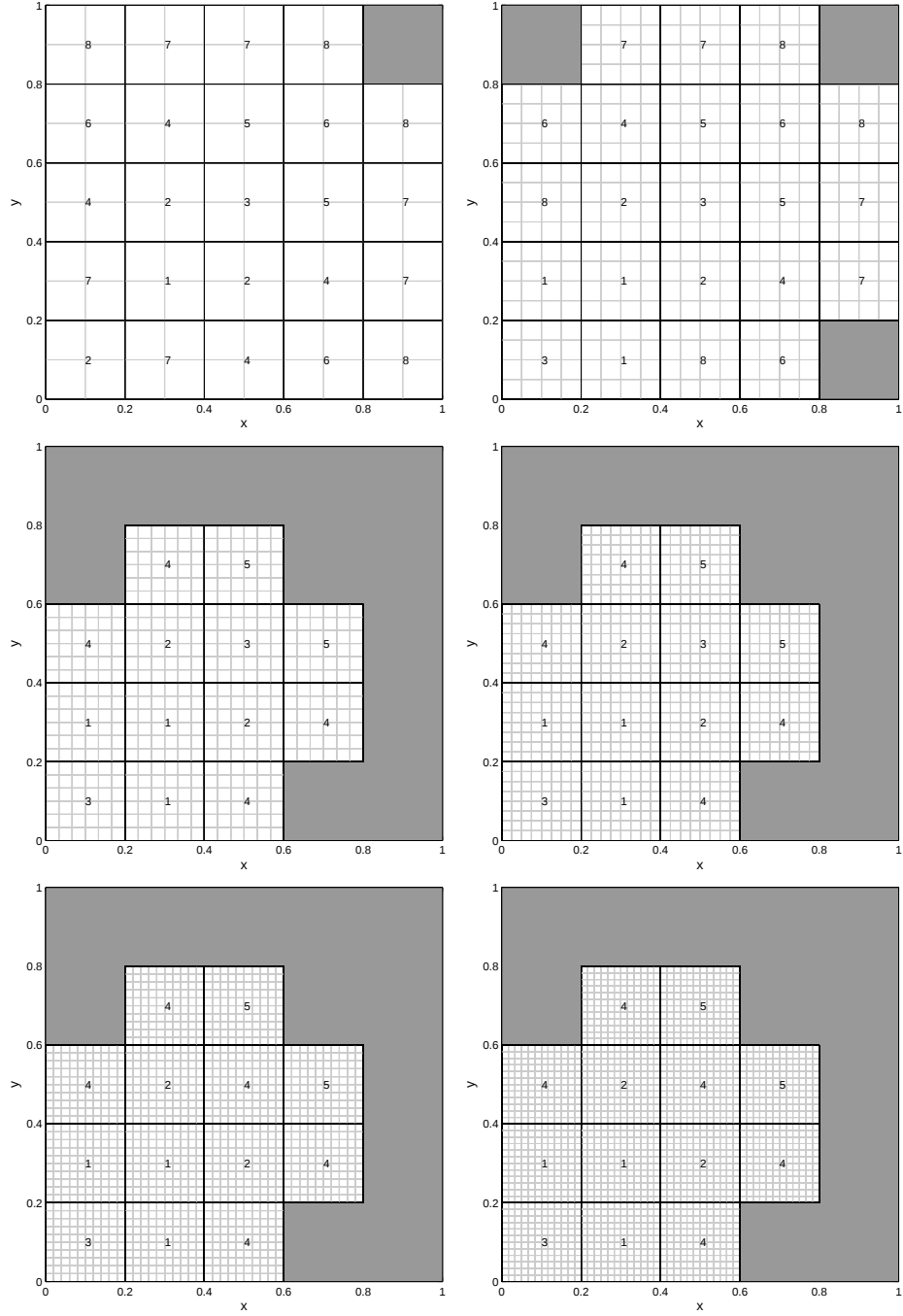


Figure 10: Adaptive modeling for the lattices 11×11 , 21×21 , ..., 61×61 for example 1. For each case the final configuration which achieves a tolerance of 5 percent in the error in the quantity of interest is shown.

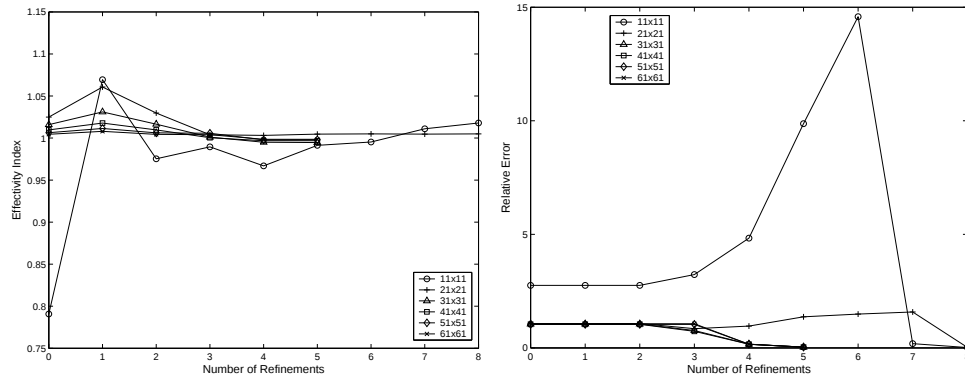


Figure 11: Effectivity indices (left) and relative errors (right) versus the number of refinements for example 1.

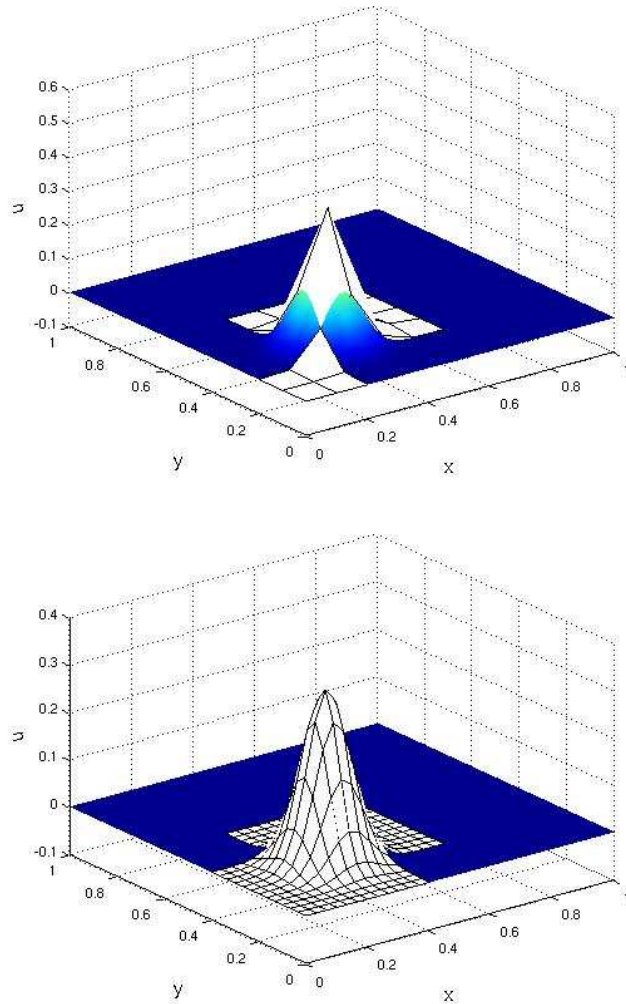


Figure 12: Solutions obtained on the reduced lattices L_3 (after iteration 3) for the 11×11 lattice (top) and the 31×31 lattice (bottom).

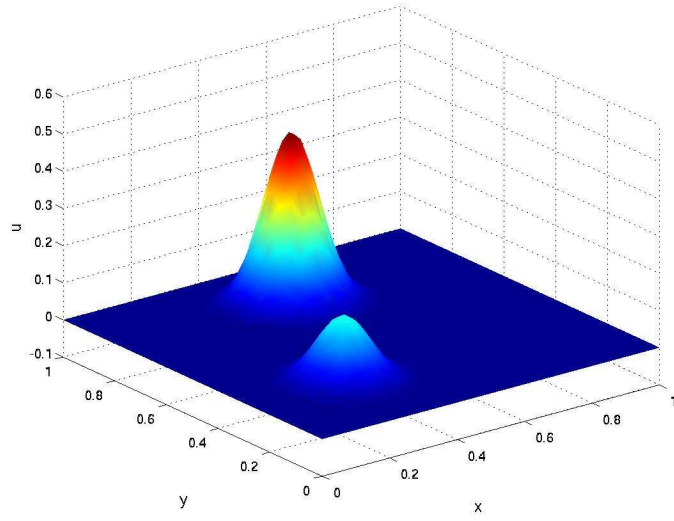


Figure 13: Accurate approximation of the continuum solution u_0 for example 2.

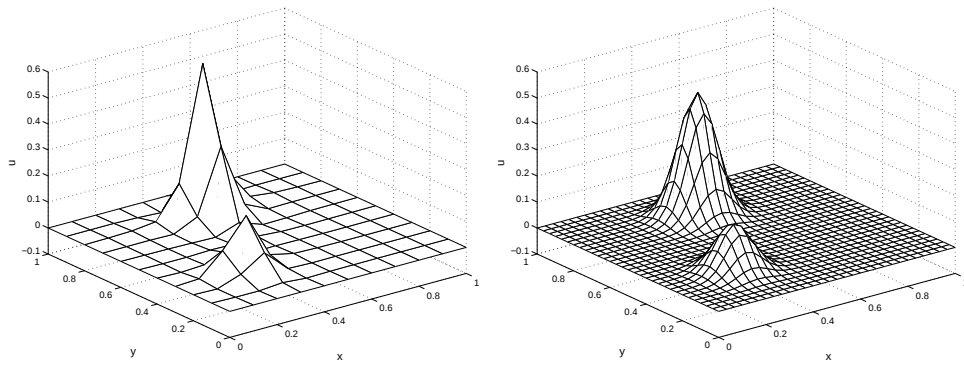


Figure 14: Lattice solutions of example 2 computed on the 11×11 and 31×31 lattices.

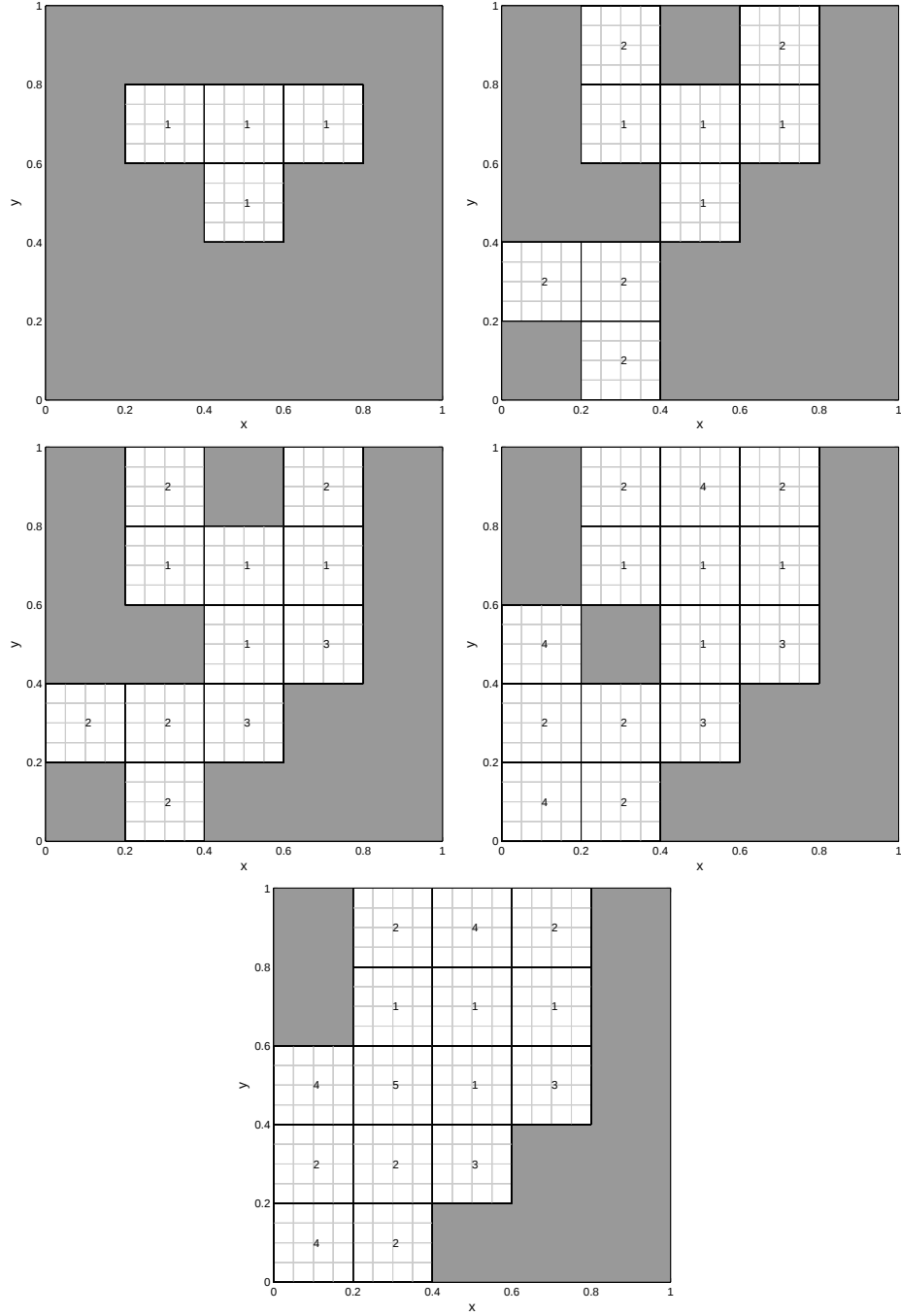


Figure 15: Sequence of surrogate models obtained by adaptive refinement for the 21×21 lattice (iterations $s = 1$ to 5). Again, the grey area represents the subregion in which the solution is obtained using the continuum model. The complementary subregion corresponds to the reduced lattice L_s . The number $l \leq s$ in the cells indicates the iteration at which the cell has been added to the lattice L_s .

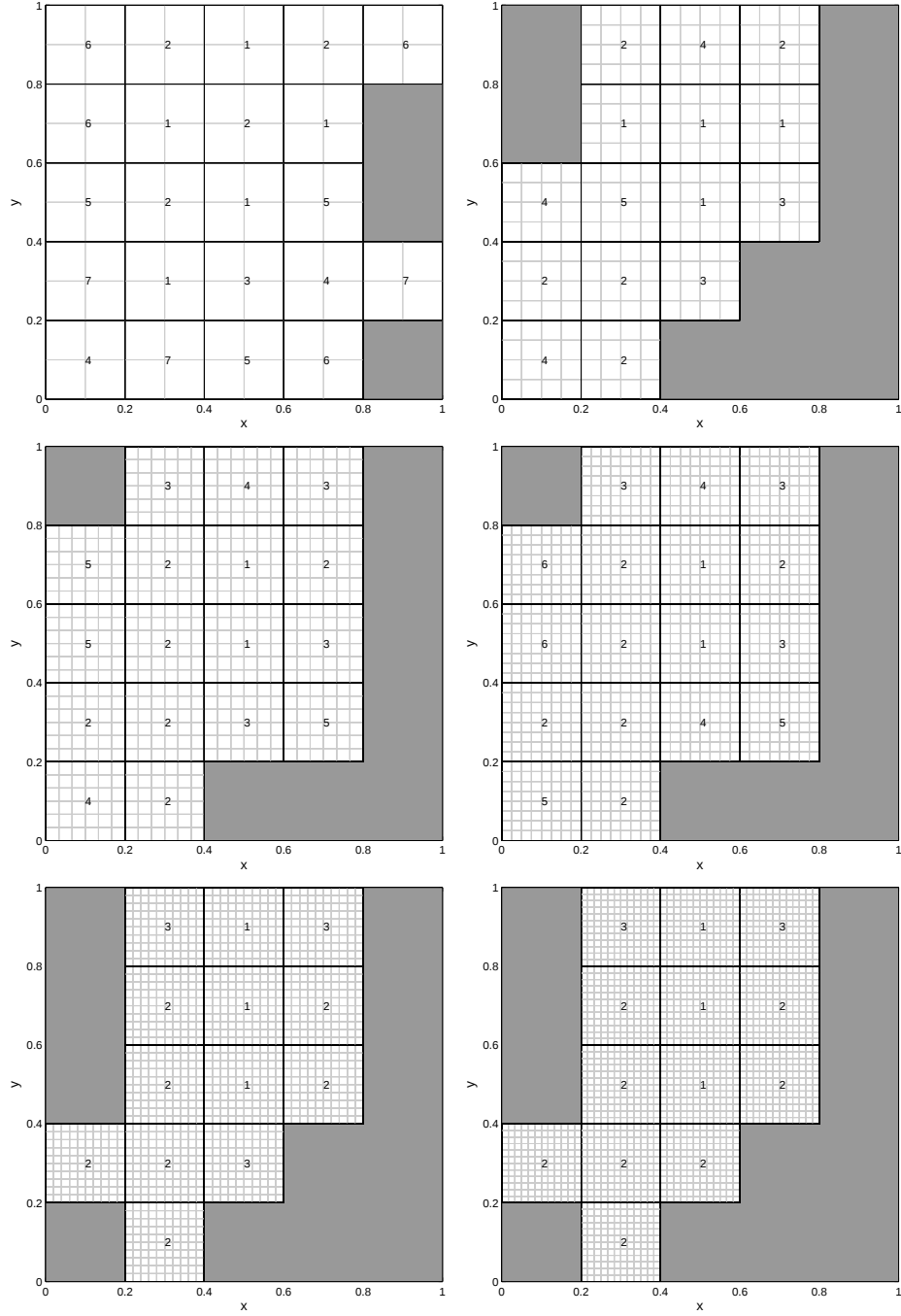


Figure 16: Adaptive modeling for the lattices 11×11 , 21×21 , $\dots$, 61×61 for example 2. For each case the final configuration which achieves a tolerance of 10 percent in the error in the quantity of interest is shown.

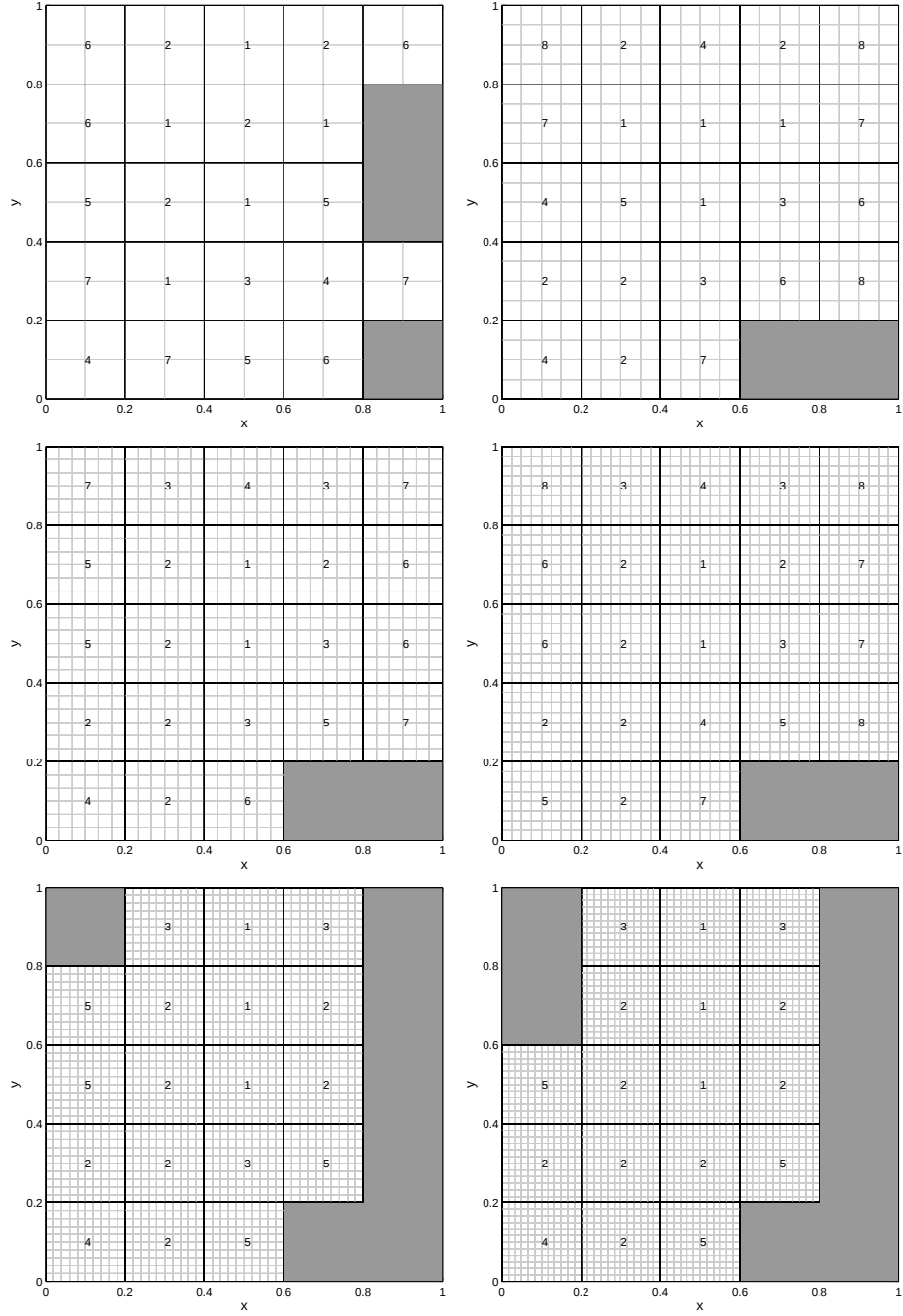


Figure 17: Adaptive modeling for the lattices 11×11 , 21×21 , $\dots$, 61×61 for example 2. For each case the final configuration which achieves a tolerance of 5 percent in the error in the quantity of interest is shown.

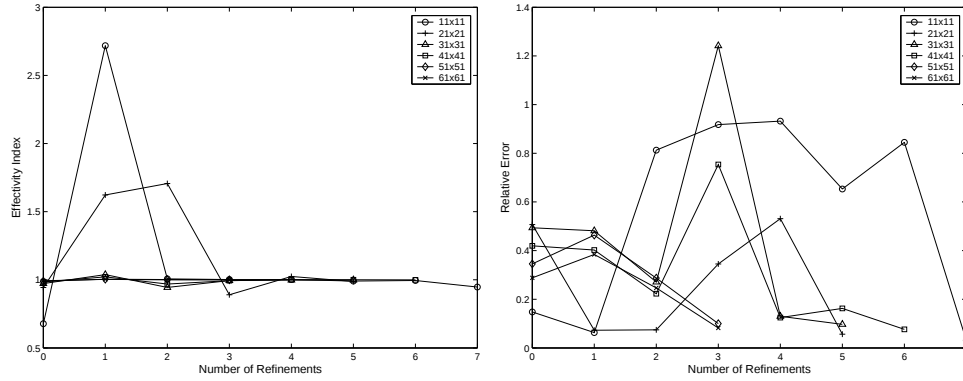


Figure 18: Effectivity indices (left) and relative errors (right) versus the number of refinements for example 2 and $\gamma_{\text{tol}} = 10$ percent.

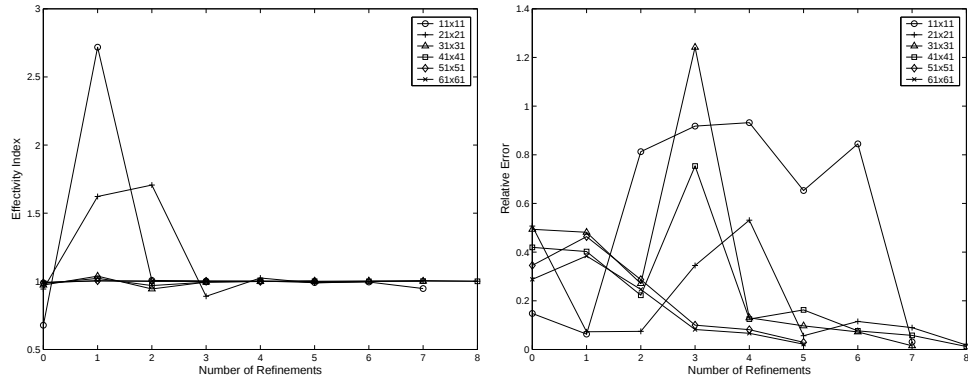


Figure 19: Effectivity indices (left) and relative errors (right) versus the number of refinements for example 2 and $\gamma_{\text{tol}} = 5$ percent.

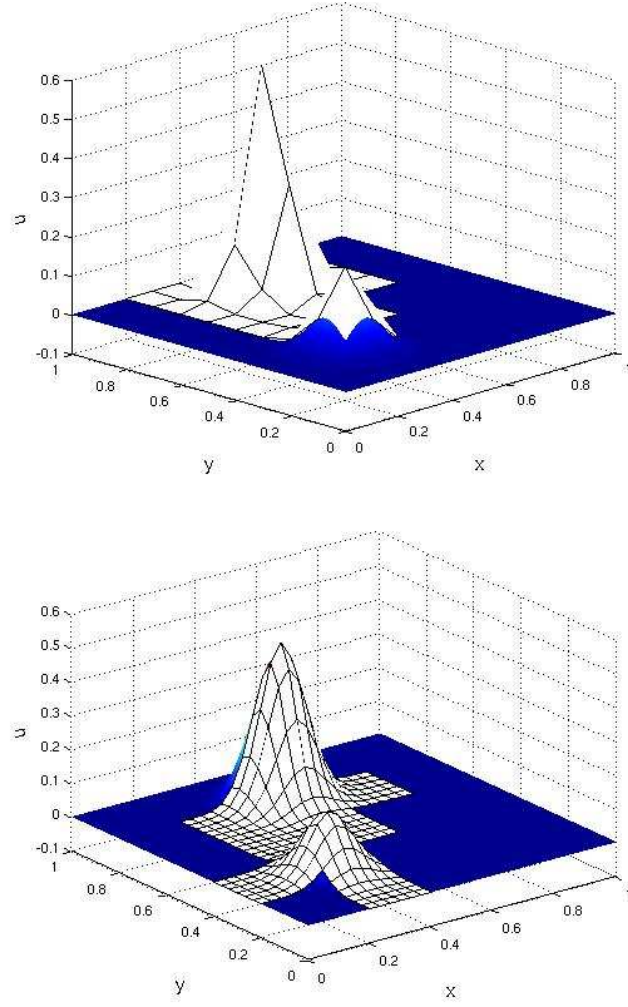


Figure 20: Solutions obtained on the reduced lattices L_2 (after iteration 2) for the 11×11 lattice (top) and the 31×31 lattice (bottom).