8 Conclusions and Outlook

Starting with a summary of what has been achieved and which points require further investigation, Section 8.1 is intended to suggest questions for future research. Section 8.2 summarizes some ideas how the multigrid solver in the complicated domain case can possibly be improved and Section 8.3 presents ideas for a multigrid coarsening strategy for discontinuous coefficients. Both these have not lead to success so far.

8.1 Summary and Open Problems

Implementation of CFE. The CFE for complicated domains presented in this thesis have been implemented except for the case of spatially varying elasticity parameters. This, however, will not require much effort. The corresponding multigrid method has also been implemented successfully with the limitations presented in Section 5.2.2. Some ideas for improvement of the multigrid method are presented below in Section 8.2.

As for the case of discontinuous coefficients, the scalar isotropic and the general linear elasticity cases have been implemented (but not the scalar anisotropic case). The development of a corresponding multigrid coarsening strategy has not been successful, some first ideas are discussed below in Section 8.3.

Both methods have not only been applied to simple artificial geometries but also to scans of actual trabecular structures with high geometric complexity.

Homogenization. Homogenization procedures have been implemented and applied for all combinations of {complicated domains, discontinuous coefficients} and {periodic, statistically periodic} fundamental cells. For complicated domains, an appropriate multigrid solver for both types of fundamental cells has also been implemented successfully, with the same limitations as before.

Again, the homogenization methods have been applied successfully to artificial geometries and samples of real trabecular bone.

Generalization of the CFE Concept. First of all, it would be useful to have a 2D CFE implementation for the cases discussed here in the same C++ framework as our 3D implementation. This should not involve methodical difficulties and would allow for easier testing of further extensions.

While we only consider 3D non-adaptive cubic meshes, a similar construction of CFE for general hexahedral, non-hexahedral or adaptive meshes is possible. This certainly requires using efficient and well-known methods for not globally uniform meshes.

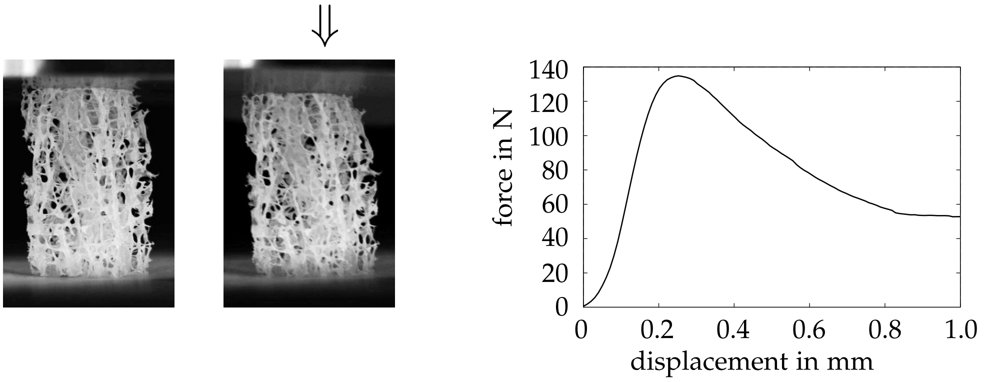

Figure 8.1. For an experimental validation of the CFE elasticity simulations for complicated domains, specimens of trabecular bone are tested in mechanical compression experiments and force is measured as a function of strain. Stiffness in the linearly elastic range (here for about 1 % of the specimen height of 12 mm) is then compared to simulation results.

If domains are described by image data, one typically uses the corresponding voxel grid and adaptivity is obtained by coarsening (unlike adaptive refinement if one starts with a coarse geometry approximation).

For 2D complicated domains, CFE for not uniformly hexahedral meshes have already been discussed in [290] and an extension to 3D should not be difficult. In contrast, CFE for discontinuous coefficients on non-uniform meshes require an appropriate interface approximation, identification of coupling conditions across the approximated interface, and finally composition of basis functions, which can be expected to be significantly more technical.

Validation. Validation of the methods used here for the elasticity case is work in progress. First, the segmentation of the image data needs to be compared to specimen volumes measured e. g. using Archimedes' principle[1] by *helium micropycnometry*, cf. [75, 332]. The elasticity method can be validated by comparing simulated macroscopic stiffnesses to those measured in compression experiments (for which the range of linearly elastic behavior needs to be identified, see Figure 8.1).

First experiments indicate that the thresholding according to [293] works well. This method determines the segmented volume by counting voxels with gray value above or below a fixed value. It seems to be unnecessary to use the CFE segmentation instead, which makes finding the threshold more than two orders of magnitude more expensive in terms of CPU time. Denoising or resampling of the dataset, however, needs to be performed with care since the structures are only a few voxels in diameter and biased errors in the segmentation will not only result in incorrect segmented volume but also in incorrect simulated mechanical results.

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[1] Named after the Greek mathematician and scientist Ἀρχιμήδης (Archimedes) who lived in the third century BC, ⋆ and † in Syracuse, Sicily [1].

8.2 Ideas for Improved Coarsening for Complicated Domains

As we have seen in Figure 7.10, some geometric situations may lead to poor multigrid convergence because coarse-grid correction introduces artificial numerical coupling. Stopping the coarsening process globally is a simple remedy (cf. Figure 7.10) which drastically decreases the efficiency of the multigrid solver. The following ideas on how this problem could be overcome are meant as suggestions for future research.

Let us propose a geometric criterion for troublesome situations in the multigrid coarsening where numerical coupling is introduced between parts of the structure whose physical coupling is only weak. Note, however, that this geometric criterion is necessary but not sufficient for a weak physical coupling of the components.

Detour-Connectedness. Recalling Figure 5.4 we observe that the support of a coarsened basis function consists of disconnected components if those components are part of disjoint subsets of the structure Ω_- or if the geodesic distance (minimal distance along paths inside Ω_-) between the components is greater than the Euclidean distance. Let us introduce the term *detour-connected* (relative to Ω_-) for sets where, between any two points, the geodesic distance (with respect to Ω_-) is not larger than the Euclidean distance plus a maximal detour ζ. If $\zeta = 0$, the set is convex.

If the imaging resolution is sufficiently high, we can assume that all supports of basis functions on the finest level are detour-connected. We can now attempt standard CFE coarsening and check whether the coarsened basis functions still have detour-connected support. If one basis function does not, a troublesome case has been detected. We can then stop the coarsening process globally and mark the current fine level as the explicit level.

We could instead stop the coarsening process only locally. This means modifying restriction and prolongation operators such that rows in the restriction matrices are left out and the coarsened problem has less DOF and no correction is prolongated from the coarse grid correction—instead of an unphysical coarse grid correction. This might make sense if detour-disconnectedness occurs only at few geometric locations and the overall convergence is not impeded by this 'better be safe than sorry' coarse grid correction. At those points, coarse grid correction could be replaced by additional smoothing steps as [53] recommends for 'pollution' of multigrid methods by reentrant corners.

Adaptive Coarsening. Another option is to determine detour-connected components of the support of basis functions. This could be achieved by assigning a 'seed node' to each DOF on the finest grid and computing geodesic distances from this seed node to neighboring DOF. During coarsening, coarse grid parent nodes could first inherit the seed of one of their descendants and geodesic distances (bounded by a detour parameter depending on the grid spacing of the current grid) could be computed for a larger neighborhood, forming the first detour-connected component of the support. If not all descendants are captured in this neighborhood, further components of the support could be introduced until all descendants are processed. For each component, a separate instance of the coarse grid node could be introduced, resulting in a 'cloning' of DOF. In further coarsening steps, this might result in further cloning, but also in 'recombination' if basis functions are found to have detour-connected support on an even coarser level. Figure 8.2 shows an example of this cloning and recombination. This approach would require bookkeeping of the different instances for the restriction and prolongation operators, either by storing additional instances separately or by using multiple copies of the grid.

Computational Complexity. Distance information can be computed using a sweeping method [326, 188], see also [80, 261, 390]. These methods usually finish within a small constant number of iterations (even though this need not be true in the worst case) with $O(n^3)$ algorithmic and memory cost if the neighborhood for which distances are computed is of size n^3 where n of course depends on the detour parameter ζ. On the finest grid, the number of nodes is $O(N^3)$ and we need one neighborhood for each node. Neighborhood and distance information is always computed on the finest grid because we need to consider the full topology information about the domain. In each coarsening step the number of grid nodes decreases roughly by a factor of 2^3, so only 1/8 of the neighborhoods (on the finest grid) need to be considered further. Their size, however, is increased by a factor 2^3. Multiple DOF for the same grid node result in multiple neighborhoods with different distance information. In the—unrealistic—worst case of 15-fold cloning, the memory requirement increases by a constant factor in each of the $O(\log N)$ coarsening steps. In total, the constants are relatively large and an implementation of this approach has not proven to be efficient.

Further Ideas. Besides this geometrically (that is, sample-specific) adapted coarsening, it may also be worth investigating the possibilities and performance of an algebraically adapted coarsening (which, most likely, depends on both specimen and

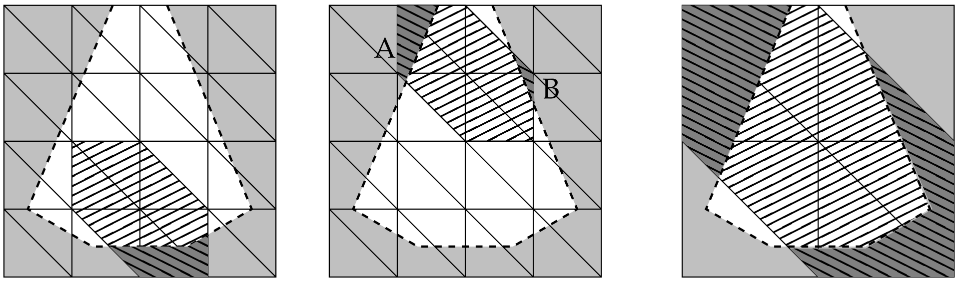

Figure 8.2. For the same example geometry as in Figure 5.4, the *left* basis function has connected support. The support of the *middle* basis function consists of two detour-disconnected components A and B, we could thus use two instances of the corresponding node. On the next coarsest level on the *right*, the two instances could be recombined because, for small nonzero detour parameter ζ, the basis function then has detour-connected support.

boundary conditions in a simulation). It may be possible (and possibly beneficial) to combine automatic coarsening methods known from algebraic multigrid solvers with the geometric information (regular structure in $\mathcal{G}^{\boxtimes}$, knowledge about interface) available. Another option could be the adaption of pseudo-L^2-projection [97] originally developed for non-nested meshes. In the terminology of [74], these could be considered (light) 'gray box' methods. If Dirichlet nodes are not visible as DOF to an algebraic coarsening procedure, these will simply be ignored and need not be treated separately.

8.3 Ideas for a Discontinuous Coefficients Coarsening Procedure

Defining a multigrid coarsening strategy for CFE for discontinuous coefficients is a difficult task that remains an open problem. A very first idea for a coarsening scheme is to simply use standard neighborhoods with standard coarsening weights 0, 1/2, and 1. In any space dimension, this clearly introduces artificial kinks in the coarsened basis functions across faces of the fine grid not present on the coarse grid.

A Geometric Coarsening Scheme in 1D. A geometrically intuitive idea for a more refined coarsening scheme can be built on the approach that coarsened basis functions should not have 'artificial' kinks on edges of the coarse grid (because a basis function constructed immediately on the coarse grid, provided that the geometry is resolved there, cannot have those kinks). This method was not found to be an effective solver strategy and its presentation is included here only for the sake of completeness.

This geometric idea can be turned in a 'slope balancing' condition from which we can determine more appropriate coarsening weights. Suppose we construct a basis function ψ_c^{CFE} on the coarse grid with the edge $[c_{\text{init}}, c_{\text{term}}] \subset \operatorname{supp} \psi_c^{\text{CFE}}$ (note that this does not imply $c \in [c_{\text{init}}, c_{\text{term}}]$ in 2D, cf. Figure 8.4, or in 3D). Then ψ_c^{CFE} has a kink on $[c_{\text{init}}, c_{\text{term}}]$ if and only if the interface intersects the edge, and the kink occurs at the

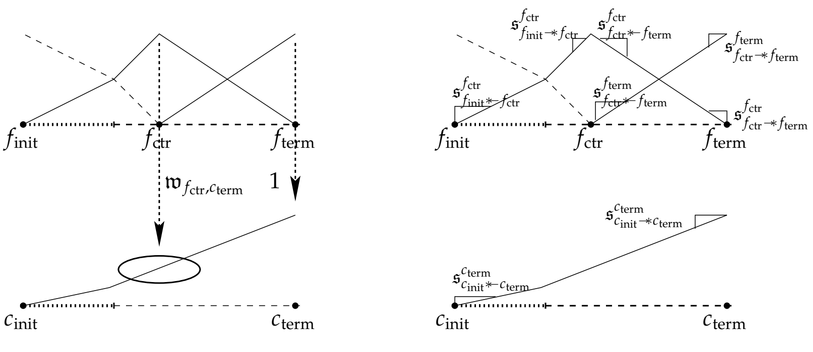

Figure 8.3. *Left:* Coarsening weights $\mathfrak{w}$ can be chosen such that the coarsened basis function does not have artificial kinks at positions where a coarse basis function would not have a kink. *Right:* For this purpose, slopes $\mathfrak{s}$ of the basis functions involved locally need to be balanced, resulting in new relevant slopes for the next coarsening step.

corresponding virtual node. In particular, there is no kink at the intermediate node $\frac{1}{2}(c_{\text{init}} + c_{\text{term}})$ which is only present on the fine grid. A coarsened basis function should also satisfy this property. Obviously, having a kink means that one-sided and other-sided slopes differ, so avoiding additonal artificial kinks can be viewed as balancing two one-sided slopes, see Figure 8.3.

Extension to 2D and 3D. For extending this coarsening scheme to more than one space dimension, first all relevant edges of the fine grid for a coarse grid node have to be identified. Note that those edges need not be incident to the coarse grid node, due to the slightly extended supports of CFE basis functions for discontinuous coefficients, also other nearby edges may play a role here. Moreover, along one such relevant edge, more than the two fine grid basis functions of the incident nodes contribute to the coarsened basis function and hence need to be considered for the slope balancing, see Figure 8.4. In total, a not necessarily symmetric local system of equations needs to be solved for the slope balancing.

The relevant slope information needs to be computed once on the finest grid, any coarsening step $l+1$ to level l then involves

1. computing coarsening weights $\mathfrak{w}_{f,c}$ based on slopes on fine grid
2. coarsening data about neighbors and relevant edges and thus determine neighborhoods $\mathcal{S}(n)^l$ for the next coarsening step
3. computing (relevant) coarsened slopes from fine slopes and coarsening weights

Notice that in absence of kinks, this slope balancing simplifies to standard coarsening. Thus the slope information only needs to be stored explicitly for basis functions affected by the interface.

Drawbacks of This Coarsening Scheme. This construction is only based on properties of the basis functions themselves. In contrast, the construction of CFE basis functions on the finest grid is based on their interpolation capabilities. This approach hence neither depends on whether we are dealing with a scalar or a vector-valued

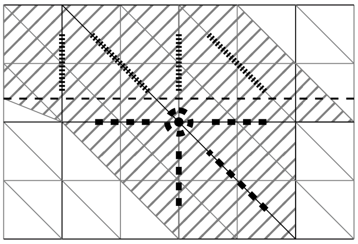

Figure 8.4. Coarsening for CFE for discontinuous coefficients requires to consider neighborhoods $\mathcal{S}$ which are larger than those for standard affine FE, resulting in larger supports for coarsened basis functions. Edges highlighed by dotted lines contribute with standard coarsening weights, additional artificial kinks need to be avoided on those edges highlighted by the thick dashed lines. The thin dashed line indicates the interface.

problem, nor does it distinguish between the isotropic and anisotropic cases. It moreover turns out that this approach leads to a violation of the partition of unity condition for the coarsened basis functions, making necessary a relaxation of the slope balancing condition.

Let us furthermore point out that kinks are avoided only across edges of the coarse grid. The CFE basis functions on the fine grid have kinks across virtual edges on the fine grid, and those virtual edges do not appear on the coarse grid (even in case of planar interfaces), as illustrated in Figure 5.7. The coarsening process does not remove such kinks by averaging them to zero (at least not near the interface). Consequently, even for simple planar interfaces, the coarsened basis functions do not coincide with those we could obtain by construction directly on the coarse grid.

Numerical Results. A CFE multigrid solver using $V_2(3,3)$ cycles for scalar isotropic discontinuous coefficients has been implemented with adaption of the coarsening weights so that the coarsened basis functions form a partition of unity. Figure 8.5 shows the convergence performance of this method compared to an SSOR-preconditioned CG solver as one example of the solvers shown in Figure 7.9, and a multigrid method using standard coarsening for affine FE on $\mathcal{G}^{\boxtimes}$ (which clearly is not a generally useful approach for discontinuous coefficients across general interfaces). Additionally, both multigrid methods cycles have also been applied as preconditioners.

We observe that the multigrid preconditioning is not effective and that performing the coarsening described above (not surprisingly) takes longer than standard coarsening. In the cases considered here, the multigrid method is effective and not significantly slower than standard multigrid, but still outperformed by the SSOR-preconditioned CG solver. Depending on geometry and (scalar) kink ratio we also encountered cases where the multigrid solver diverged.

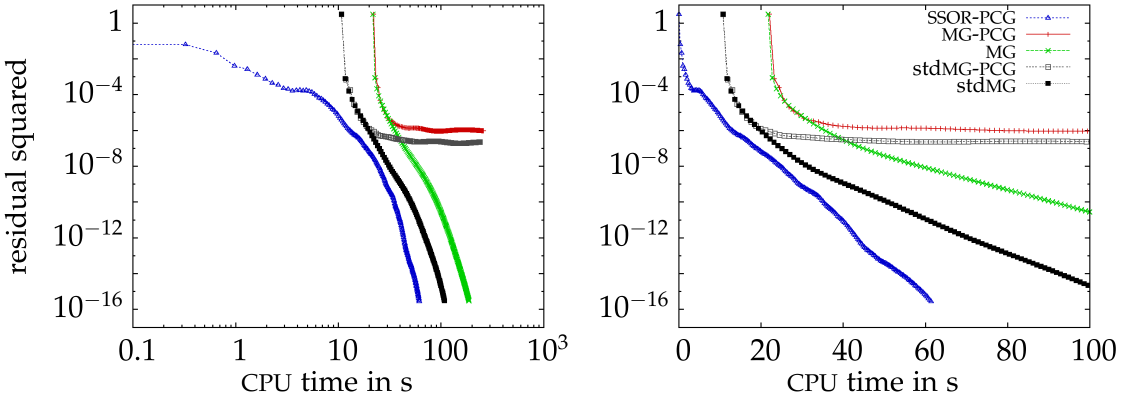

Figure 8.5. The plots compare the solver convergence of multigrid solvers and preconditioning using the coarsening scheme described here and standard affine FE coarsening, using a logarithmic and a linear time scale. The same bone interfaces as in Figure 7.9 were used, the scalar kink ratio was again $\kappa = 42$. An SSOR-preconditioned CG solver outperforms all multigrid-based solvers in this case.

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