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COMPUTATIONALLY EFFICIENT ALGORITHMS FOR EVALUATION OF STATISTICAL DESCRIPTORS

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Abstract: *Homogenization methods are becoming the most popular approach to modelling of heterogeneous materials. The main principle is to represent the heterogeneous microstructure with an equivalent homogeneous material. When dealing with the complex random microstructures, the unit cell representing exactly periodic morphology needs to be replaced by a statistically equivalent periodic unit cell (SEPUC) preserving the important material properties in the statistical manner. One of the statistical descriptors suitable for SEPUC definition is the lineal path function. It is a low-order descriptor based on a more complex fundamental function able to capture certain information about the phase connectedness. Its main disadvantage is the computational cost. In this contribution, we present the reformulation of the sequential C code for evaluation of the lineal path function into the parallel C code with Compute Unified Device Architecture (CUDA) extensions enabling the usage of computational potential of the NVIDIA graphics processing unit (GPU).*

Keywords: ***Lineal path function, homogenization, statistically equivalent periodic unit cell, graphics processing unit.***

1. Introduction

Modelling of random heterogeneous materials is a multi-disciplinary problem with a wide range of relevant engineering applications. The unifying theoretical framework is provided by homogenization theories, which aim at the replacement of the heterogeneous microstructure with an equivalent homogeneous material, e.g. Torquato (2002). Currently, two main approaches are available: (i) computational homogenization and (ii) effective media theories. While the first class of methods studies the distribution of local fields within a typical heterogeneity pattern using a numerical method, the second group estimates the response analytically on the basis of limited geometrical information (e.g. the volume fractions of constituents) of the analysed medium.

It is generally accepted that detailed discretisation techniques, and the Finite Element Method (FEM) in particular, remain the most powerful and flexible tools available. Despite of the tedious computation time, it provides us details of local stress and strain fields. Moreover, it is convenient to characterize the material heterogeneity by introducing the concept of a Periodic Unit Cell (PUC) (Vorel, 2009) or Statistically Equivalent Periodic Unit Cell (SEPUC), see Zeman and Šejnoha (2007); Vorel et al. (2012) for more details. On the other hand, if only the overall (macroscopic) response is demanded variable, it is sufficient to introduce structural imperfections in a cumulative sense using one of the averaging schemes, e.g. the Mori-Tanaka method (Vorel and Šejnoha, 2009). If the effective material parameters of complex microstructure (see Figure 1) are demanded, the homogenization technique based on the SEPUC can be utilized. Furthermore, this approach allows us to reduce the computation cost by generating smaller unit cell describing the real structure. The generation of the SEPUC is based on optimization of an appropriate statistical descriptor. One most commonly used group of descriptors embodies a set of general n-point probability functions, applicable to an arbitrary two-phase composite. A different statistical function deserves attention when phase connectivity information is to be captured in more

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detail, as e.g. for medium in Figure 1. Therefore we focus here on usage of the lineal path function. The principal drawback concerns its evaluation, which is non-negligible time-consuming, especially when evaluated many times within the optimization process. Hence, we present an accelerated implementation of the lineal path function on the GPU. The following section details the definition of the lineal path

Fig. 1: Three cuts through trabecular bone microstructure obtained by micro Computed Tomography (Jiroušek et al., 2008)

function. The Section 3. discusses its algorithmic formulation and Section 4. presents the resulting speed-up obtained at GPU in comparison with the sequential CPU formulation together with concluding remarks.

2. Lineal path function

The lineal path function (Lu and Torquato, 1992) is one of the low-order microstructural descriptors based on a more complex fundamental function which contains more detailed information about phase connectedness and hence certain information about long-range orders (Zeman, 2003).

The fundamental function can defined as

$$\lambda_r(\mathbf{x}_1, \mathbf{x}_2, \alpha) = \begin{cases} 1, \text{ if } \mathbf{x}_1\mathbf{x}_2 \subset D_r(\alpha), \\ 0, \text{ otherwise,} \end{cases} \tag{1}$$

i.e., a function which equals to 1 when the segment $\mathbf{x}_1\mathbf{x}_2$ is contained in the phase r for the sample α and zero otherwise. The lineal path function, denoting the probability that the $\mathbf{x}_1\mathbf{x}_2$ segment lies in the phase r, then follows directly from the ensemble averaging of this function

$$L_r(\mathbf{x}_1, \mathbf{x}_2) = \overline{\lambda_r(\mathbf{x}_1, \mathbf{x}_2, \alpha)}. \tag{2}$$

Under the assumptions of statistical homogeneity and isotropy, the function simplifies to

$$L_r(\mathbf{x}_1, \mathbf{x}_2) = L_r(\mathbf{x}_1 - \mathbf{x}_2) = L_r(\|\mathbf{x}_1 - \mathbf{x}_2\|). \tag{3}$$

Obviously, if the points $\mathbf{x}_1$ and $\mathbf{x}_2$ coincide, the lineal path function takes the value of volume fraction of the phase r. On the other hand, for points $\mathbf{x}_1$ and $\mathbf{x}_2$ that are far apart the lineal path function vanishes.

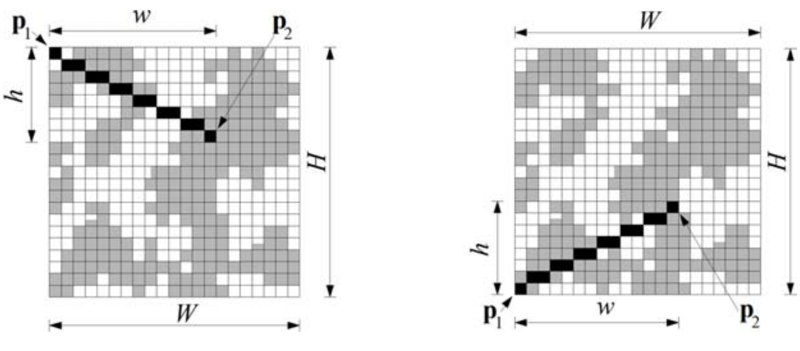


Fig. 2: Schema of the lineal path function

3. Algorithmic formulation

The generation of SEPUC is usually based on digital images, which are discretised representation of a studied medium. The segments are then defined as a set of pixels connecting two pixels $\mathbf{p}_1$ and $\mathbf{p}_2$ with the coordinates within the image $\mathbf{p}_i = (w, h)$, and , where W and H are the dimensions of the image (see Figure 2). The sets of pixels for segments starting in $\mathbf{p}_1 = (1, 1)$ and ending in $\mathbf{p}_2 = (w, h)$ are obtained by algorithm given in Bresenham (1965). The group of segments is complemented by the ones starting in $\mathbf{p}_1 = (1, H)$ and ending in $\mathbf{p}_2 = (w, h)$ to cover all possible lengths and orientations within the image. Once having the defined segments, the computation of lineal path function involve simple translations of each segment throughout the image and the comparison whether all pixels of the segment at a given position correspond to image pixels with the value representing the investigated phase.

Since the generation of segments can be done only once for a given image size, this part of the code does not necessarily need to be so fast. The crucial part of the code is the translation of the segment and the comparison with the image, which is called repeatedly for any new image created during the optimization of the SEPUC. Having a single CPU, the translations and comparisons needs to be performed sequentially, see Figure 3. Last years witnessed increasing popularity of parallel computations on GPUs.

```
Generate_Segments();
for( i=0; i < nsegments; i++ ){
   for( j=0; j < npixels; j++ ){
      Is_Inside();
   }
}
```

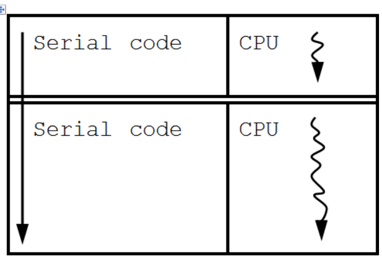


Fig. 3: Schema of the sequential code

The reason is the high performance at relatively low cost. Moreover, the CUDA simplifies the GPU-based software development by using the standard C language, see NVIDIA Corporation (www). We used the high number of simple GPU threads to compute the translations and comparisons of segments simultaneously, see Figure 4.

```
Generate_Segments();


// Parallel kernel
Is_Inside<<< >>>(nsegments,npixels);

```

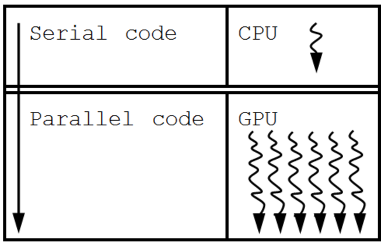
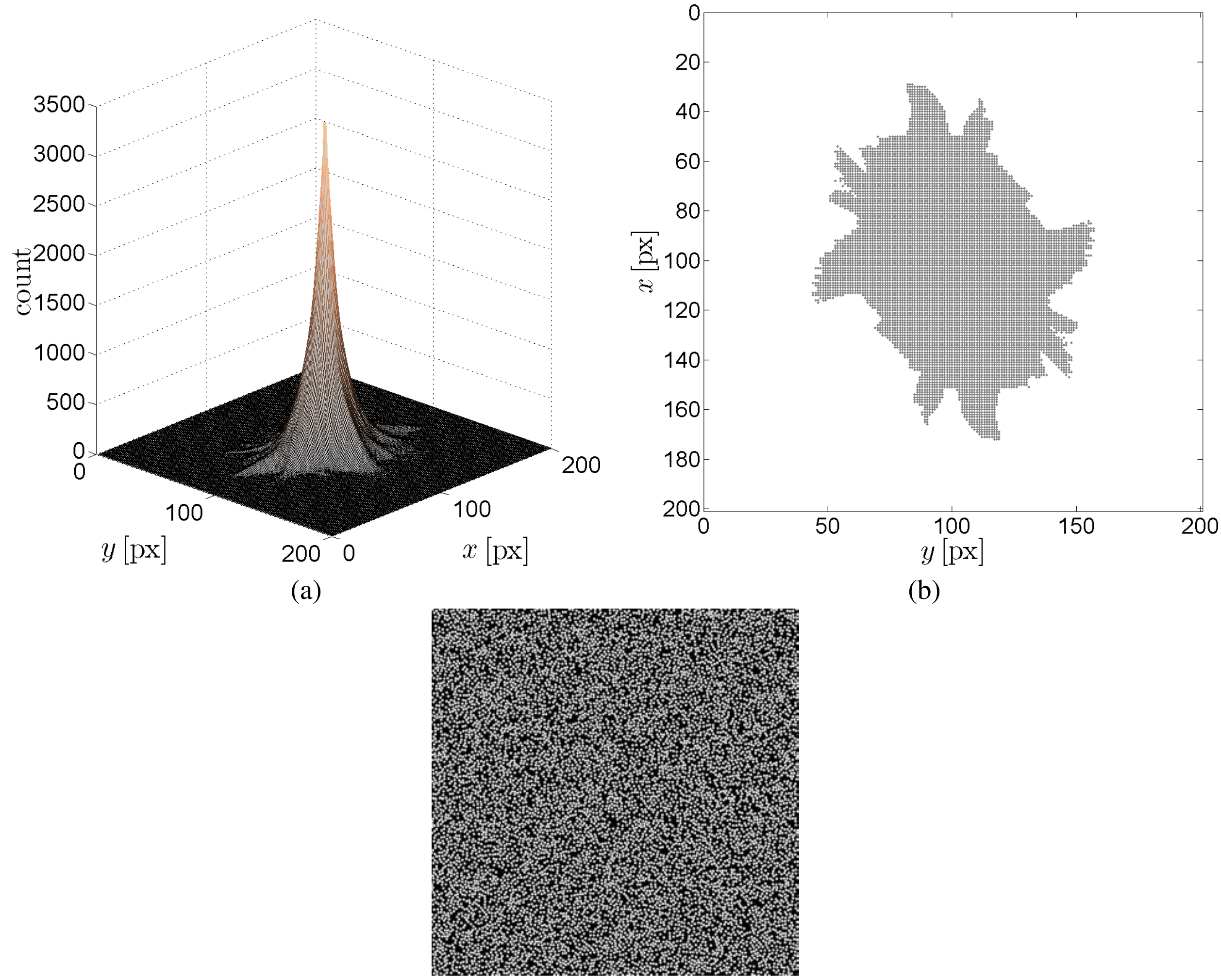


Fig. 4: Schema of the parallel code

4. Conclusions

We have compared the sequential variant of lineal path function calculation on a single CPU with the parallel one using the GPU. The particular computations were performed on INTEL Core i7 CPU 950 @ 3.07 GHz, 12 GB RAM, GPU - NVIDIA QUADRO 4000 with Microsoft Windows Enterprise SP 1 operating system and the CUDA v. 4.0 compute capability. The efficiency of GPU parallelism was demonstrated on evaluation of lineal path function for 10 two-dimensional images with the size varying from 50x50 px to 500x500 px, see Figure 5(c). Two distinct calculations of lineal path function were considered. The originally developed algorithm covering all possible segments in the domain and enhanced method with constraint of first zero segment in given direction. Table 1 shows the amount of time necessary for one evaluation of lineal path function depending on the image size and chosen method.



(c)

Fig. 5: (a) Lineal path function, (b) lineal path function (view X-Y), (c) testing image 500x500 px

One can see that for very small images, the usage of CPU outperforms the GPU because of additional time spent by copying the data from main memory RAM to GPU memory. Nevertheless, the parallelism of GPU gains for images larger than 50x50 px and the time savings increase rapidly.

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Standard				*Enhanced*				
D/ML [px]/[px]	GPU [s]	CPU [s]	**ratio**	D/ML [px]/[px]	GPU [s]	CPU [s]	**ratio**	**overall speedup**
50/50	0.179	0.328	**1.83**x	50/50	0.156	0.265	**1.69**x	**2.10**x
100/100	1.075	4.617	**4.29**x	100/100	0.722	2.371	**3.28**x	**6.39**x
150/150	3.957	21.653	**5.47**x	150/150	1.954	8.018	**4.10**x	**11.08**x
200/200	10.209	66.425	**6.51**x	200/200	3.621	14.742	**4.07**x	**18.34**x
250/250	22.276	169.245	**7.59**x	250/250	6.427	27.612	**4.29**x	**26.33**x
300/300	43.429	357.022	**8.22**x	300/250	8.413	42.338	**5.03**x	**42.44**x
350/350	76.644	649.195	**8.47**x	350/250	10.909	63.304	**5.80**x	**59.51**x
400/400	127.841	1127.897	**8.82**x	400/250	13.481	84.287	**6.25**x	**83.67**x
450/450	209.693	1821.911	**8.69**x	450/250	18.608	122.569	**6.59**x	**97.91**x
500/500	315.951	2846.712	**9.01**x	500/250	21.145	139.698	**6.61**x	**134.64**x

Tab. 1: Comparison of CPU and GPU performance (D=dimension of testing image in pixels, ML=maximal length of segment in pixels)

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