Running Large-Scale Ultrasound Simulations on Piz Daint with 512 Pascal GPUs

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ABSTRACT

This paper presents a novel local domain decomposition for full-wave ultrasound propagation simulations with a custom bell function which ensures the numerical error stays below 10^{-3} while enabling almost ideal strong scaling. Realistic benchmarks with 512 Nvidia P100 GPUs in the best EU supercomputer Piz Daint achieved efficiency between 90 and 100% with a speed-up over 100 and computational cost reduction by a factor of 12 compared to 1024 Haswell cores.

KEYWORDS

Ultrasound simulations, Local domain decomposition, Pseudospectral methods, k-Wave toolbox, GPU, Piz Daint.

1 INTRODUCTION

Ultrasound simulation is a critical component of model-based treatment planning for ultrasound therapy [9]. However, the domain are typically thousands of wavelengths in size, leading to large numerical models with billions of unknowns.

Pseudospectral time domain (PSTD) and k-space methods, in which spatial gradients are calculated using the Fourier collocation spectral method, have been shown to be particular efficient for solving these large scale problems, due their exponential error convergence with grid density [10], [11]. However, the computational performance of methods that utilize 3D fast Fourier transforms (FFTs) across the global domain is inhibited by the requisite globally-synchronizing all-to-all data exchanges, see Fig. 1 and [5], [7]. The communication bottleneck is even more striking on GPU-accelerated clusters where the communication part may easily reach 95% of computational time [3].

2 PROPOSED METHOD

Our approach to overcome the bottleneck of global communication in Fourier spectral methods is to divide the global domain into local subdomains, and perform calculations using FFTs only on the local domain (i.e., using a local Fourier basis) [4, 6]. Local calculations are then interleaved with the exchange of data only between neighboring subdomains within an overlap region, which significantly reduces the communication overhead. The accuracy of the spectral gradient calculations is maintained by forcing the subdomains to be periodic through multiplication of the local data by a bell function [1].

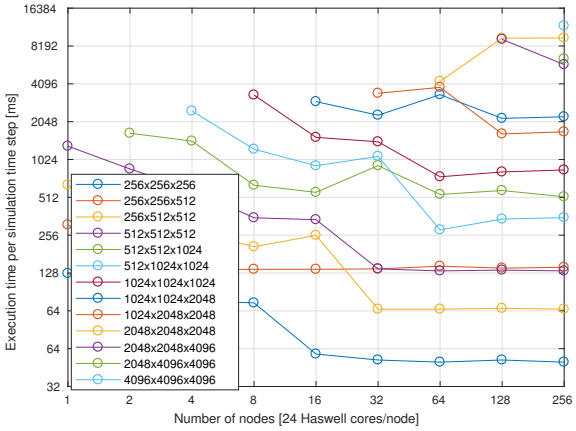

Figure 1: Strong scaling of ultrasound simulations with slab-based global domain decomposition introduced in FFTW[2] on the Salomon cluster with 6144 Haswell cores and 56Gb Infiniband network. Domain sizes vary between 256^3 and 4096^3 grid points.

However, giving up the global gradient calculation naturally leads to an accuracy loss which linearly increases anytime the wave crosses a subdomain boundary. Fortunately, the trade-off between the computational efficiency and the numerical accuracy can be controlled by two parameters: (1) the shape of the bell function, and (2) the size of the overlap region, see Fig. 2. Here, we used numerical optimization to design the shape of the bell function to minimize the numerical error introduced by the decomposition. An overlap size of 8 grid points is then sufficient to maintain the L∞ error below 0.1% even after the wave has crossed 8 subdomain boundaries. For 3D decompositions, this corresponds to $9^3 = 729$ local subdomains. If a higher number of subdomains is needed to distribute the work over more nodes (CPU/GPU), the overlap region may be extended, e.g., an overlap size of 16 is sufficient for $17^3 = 4913$ subdomains reaching the number of GPUs on the Piz Daint supercomputer. Let us also note the typical measurement error in clinical applications is around 1%, thus, even smaller overlap size may be applicable [8].

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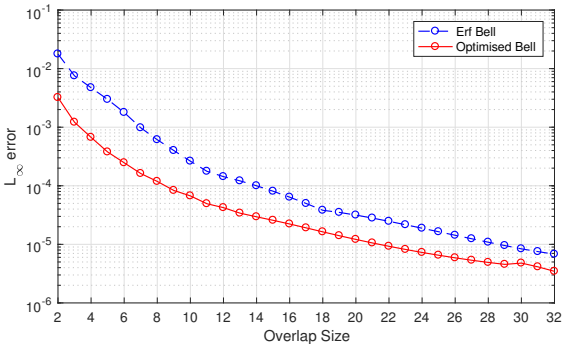

Figure 2: The L∞ error introduced by crossing a subdomain boundary in dependence on the overlap size and the bell function shape.

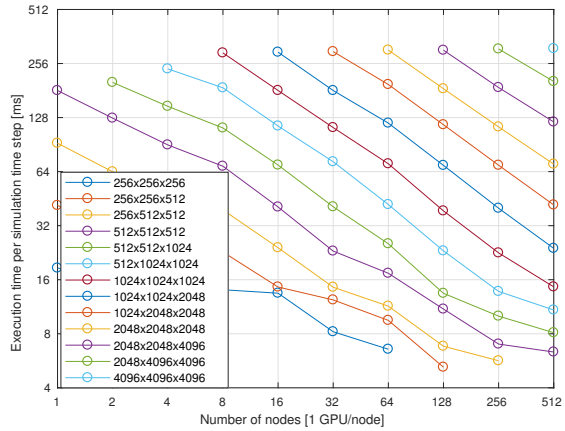

Figure 3: Strong scaling of ultrasound simulations with local domain decomposition and overlap size of 8 on Piz Daint with 512 GPUs and aries network. Domain sizes between 256^3 and 4096^3 grid points.

3 EXPERIMENTAL RESULTS

The implementation of the local domain decomposition was developed in C++ with CUDA 8.0 and OpenMPI library. The experimental measurements were conduced on the CSCS Piz Daint system[1] equipped with Nvidia Pascal P100 GPUs. The strong scaling presented in Fig. 3 shows an excellent scaling up to 512 GPUs even for small domains (e.g., a domain of 512^3 grid points is divided into tiny subdomains of 64^3 when executed on 512 GPUs). Fig. 4 shows the box plot of achieved speedups every time the number of subdomains was doubled for the overlap size of 4 and 16. While for the overlap size of 4, the achieved speedups are closed to 2 for large domains (efficiency nearly 100% with fully overlapped communication), the bigger overlap of 16 causes the maximum speed-up touching 1.8 (efficiency of 90%).

[1] http://www.cscs.ch/computers/piz_daint/index.html

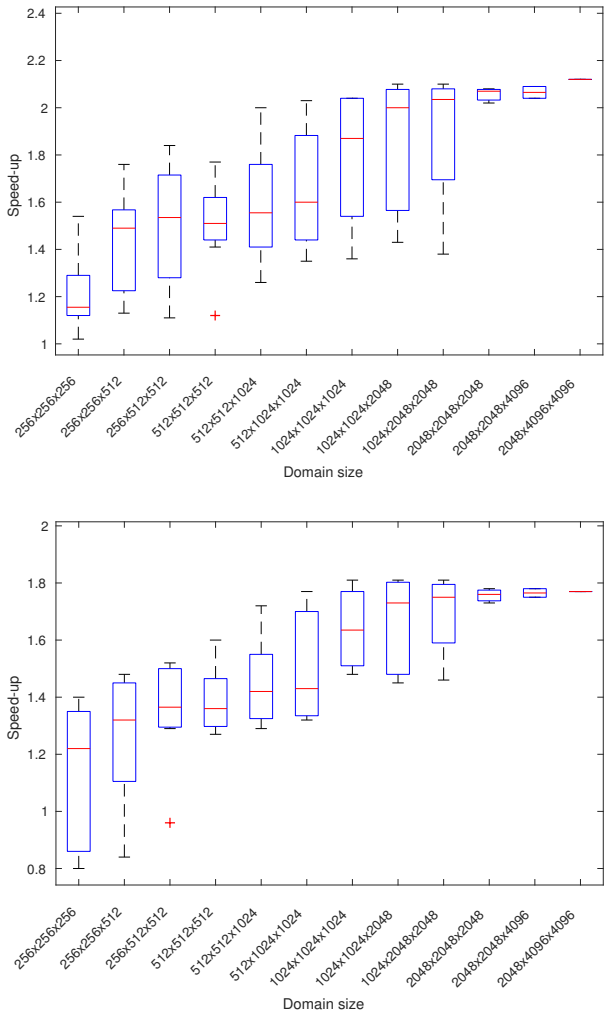

Figure 4: Gradient of scaling curves (speed-up when doubling the number of subdomains/GPUs) for overlap sizes of 4 (top) and 16 (bottom) on Piz Daint.

4 CONCLUSIONS

This paper has presented a novel domain decomposition for large-scale ultrasound simulations which has allowed some of the largest ultrasound simulations to date to be conducted. By numerical optimization of the bell function and careful overlap size selection, we achieved efficiency between 90 and 100% for 512 GPUs of Piz Daint while keeping the numerical error at aceptable levels around 0.1%.

The main contribution of this paper is, however, the possibility to fully exploit GPUs in cluster environment, impractical with standard global domain decompositions. Comparing with the global slab decomposition on running on a Haswell based cluster, the GPU solution offers more than 100× higher performance and 12× lower simulation cost.

5 ACKNOWLEDGEMENT

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