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### 3D frequency-domain seismic modeling with a Parallel BLR multifrontal direct solver

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#### SUMMARY

Three-dimensional frequency-domain full waveform inversion (FWI) of fixed-spread data can be efficiently performed in the visco-acoustic approximation when seismic modeling is based on a sparse direct solver. We present a parallel algebraic Block Low-Rank (BLR) multifrontal solver which provides an approximate solution of the time-harmonic wave equation with a reduced operation count, memory demand, and volume of communication relative to the full-rank solver. We analyze the parallel efficiency and the accuracy of the solver with a realistic FWI case study from the Valhall oil field.

#### INTRODUCTION

Seismic modeling and full waveform inversion (FWI) can be performed either in the time domain or in the frequency domain (e.g., Virieux and Operto, 2009). In the frequency domain, seismic modeling consists of solving an elliptic boundary-value problem, which can be recast in matrix form as a system of linear equations where the solution (i.e., the monochromatic wavefield) is related to the right-hand side (i.e., the seismic source) through a sparse impedance matrix, whose coefficients depend on frequency and subsurface properties (e.g., Marfurt, 1984). One distinct advantage of the frequency domain is to allow for a straightforward implementation of attenuation in seismic modeling (e.g., Toksöz and Johnston, 1981). Second, it provides a suitable framework to implement multi-scale FWI by frequency hopping, that is useful to mitigate the nonlinearity of the inversion (e.g., Pratt, 1999). Third, monochromatic wavefields can be computed quite efficiently for multiple sources by forward/backward substitutions if the linear system can be solved with a sparse direct solver based on the multifrontal method (Duff and Reid, 1983). However, the LU factorization of the impedance matrix that is performed before the substitution step generates fill-in, which makes this pre-processing step memory demanding. Dedicated finite-difference stencils of local support (Operto et al., 2014) and fill-reducing matrix ordering based on nested dissection (George and Liu, 1981) are commonly used to minimize this fill-in.

This limitation motivates to compute approximate solutions of the linear system by exploiting the low-rank properties of elliptic partial differential operators (Wang et al., 2011). Several approaches exist to achieve this objective. The Block Low-Rank (BLR) approach (Amestoy et al., 2015b) can be easily and efficiently embedded in a multifrontal solver. In Weisbecker et al. (2013), we presented its potential in a sequential environment using the BLR solver. In this study, we generalize the approach to a parallel context and present the chal-

lenges that need to be overcome to preserve the efficiency of the solver on modern distributed-memory machines with multicore processors. In the first part, we review the main features of the parallel BLR multifrontal solver. Second, seismic modeling in a subsurface model of the Valhall oil field in the 3.5Hz-10Hz frequency band gives quantitative insights on the memory and operation count savings provided by the BLR approach. We also present the parallel performance of the solver. The relevance of the BLR approach to perform FWI of real ocean-bottom cable data recorded in the Valhall oil field is illustrated in a companion abstract (Amestoy et al., 2015a).

#### PARALLEL BLOCK LOW-RANK MULTIFRONTAL METHOD

##### Parallel Multifrontal method

The multifrontal method was first introduced by Duff and Reid (1983). Being a direct method, it computes the solution of a sparse system  $Ax = b$  by means of a factorization of  $A$  under the form  $A = LU$  (in the unsymmetric case). This factorization is achieved through a sequence of *partial factorizations*, performed on dense matrices, called *fronts*. With each front are associated two sets of variables: the *fully-summed (FS) variables*, whose corresponding rows and columns of  $L$  and  $U$  are computed within the current front, and the *non fully-summed (NFS) variables*, which receive updates resulting from the elimination of FS variables. At the end of each partial factorization, the partial factors  $[L_{11}L_{21}]$  and  $[U_{11}U_{12}]$  are stored apart and a Schur complement referred to as a contribution block (CB) is held in a temporary memory area called *CB stack*, whose maximal size depends on several parameters. As the memory needed to store the factors is incompressible (in full-rank), the *CB stack* can be viewed as an overhead whose peak has to be minimized. The structure of a front before and after partial factorization is shown in Fig. 1. The computa-

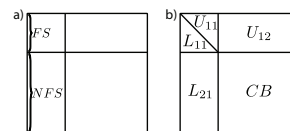


Figure 1: A front before (a) and after (b) partial factorization.

tional and memory requirements for the complete factorization strongly depend on how the fronts are formed and on the order in which they are processed. Reordering techniques such as nested dissection are used to ensure the efficiency of the process: a so-called *elimination tree* (Schreiber, 1982) is created, with a front associated with each of its nodes. Any post-order traversal of this tree gives equivalent properties in terms of factors memory and computational cost.

## Seismic modeling with a Block Low-Rank direct solver

In a parallel environment, two kinds of parallelism, referred to as *tree parallelism* and *node parallelism*, are exploited (Fig. 2). In *tree parallelism*, fronts in different sub-trees are processed by different processes, while in *node parallelism*, large enough fronts are mapped on several processes: the master process is assigned to process the fully-summed rows and is in charge of organizing computations; the non fully-summed rows are distributed following a one-dimensional row-wise partitioning, so that each slave holds a range of rows.

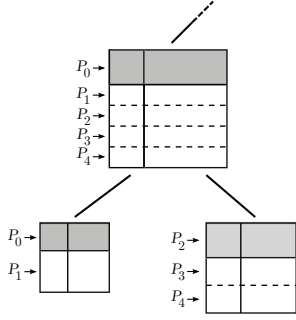


Figure 2: Illustration of tree and node parallelism. The shaded part of each front represents its fully-summed rows. The fronts are row-wise partitioned in our implementation, but column-wise partitioning is also possible.

### Block Low-Rank (BLR) matrices

A flexible, efficient technique can be used to represent fronts with low-rank sub-blocks based on a storage format called Block Low-Rank (BLR, see Amestoy et al. (2015b)). Unlike other formats such as  $\mathcal{H}$ -matrices (Hackbusch, 1999) and HSS matrices (Xia et al., 2009), the BLR one is based on a flat, non-hierarchical blocking of the matrix which is defined by conveniently clustering the associated unknowns. A BLR representation of a dense matrix  $F$  is shown in equation (1) where  $p$  sub-blocks have been defined. Sub-blocks  $\tilde{B}_{ij}$  of size  $m_i \times n_j$  and numerical rank  $k_{ij}^\varepsilon$  are approximated by a low-rank product  $X_{ij}Y_{ij}^T$  at accuracy  $\varepsilon$ , when  $k_{ij}^\varepsilon(m_i + n_j) \leq m_in_j$  is satisfied.

$$\tilde{F} = \begin{bmatrix} \tilde{B}_{11} & \cdots & \tilde{B}_{1p} \\ \vdots & \ddots & \vdots \\ \tilde{B}_{p1} & \cdots & \tilde{B}_{pp} \end{bmatrix} \quad (1)$$

In order to achieve a satisfactory reduction in both the complexity and the memory footprint, sub-blocks have to be chosen to be as low-rank as possible (e.g., with exponentially decaying singular values). This can be achieved by clustering the unknowns in such a way that an *admissibility condition* (Bebendorf, 2008) is satisfied. This condition states that a sub-block  $\tilde{B}_{ij}$ , interconnecting variables of  $i$  with variables of  $j$ , will have a low rank if variables of  $i$  and variables of  $j$  are *far away* in the domain, intuitively, because the associated variables are likely to have a weak interaction. In practice, the sub-graphs induced by the FS variables and the NFS variables are algebraically partitioned with a suitable strategy.

### Parallel BLR multifrontal solver

A BLR multifrontal solver consists in approximating the fronts

with BLR matrices. BLR representations of  $[L_{11}U_{11}]$ ,  $L_{21}$ ,  $U_{12}$  and CB are computed separately. The partial factorization occurring at each front of the multifrontal method is then adapted to benefit from the compressions using low-rank products instead of full-rank standard ones. An example of a BLR partial factorization algorithm is given in Algorithm 1; many variants can be easily defined, depending on the position of the Compress operation. For sake of clarity, we present the version with only one process mapped on the front. For fronts with several processes, the Factor task is done on the master, while each slave performs the Solve, Compress and Update tasks on their respective block of rows.

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#### Algorithm 1 Partial dense BLR LU factorization.

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1:   Input: a  $m \times m$  block matrix  $A$  of size  $n$ ;  $A = [A_{i,j}]_{i=1:m,j=1:m}$ ; with  $p$  the number of blocks to eliminate
2:   for  $k = 1$  to  $p$  do
3:     Factor:  $A_{k,k:m} = L_{k,k}U_{k,k:m}$ 
4:     for  $i = k + 1$  to  $m$  do
5:       Solve (compute L):  $A_{i,k} \leftarrow A_{i,k}U_{k,k}^{-1}$ 
6:       Compress:  $A_{k,i} \approx X_{k,i}Y_{k,i}^T$  and  $A_{i,k} \approx X_{i,k}Y_{i,k}^T$ 
7:     end for
8:     for  $i, j = k + 1$  to  $m$  do
9:       Update:  $A_{i,j} \leftarrow A_{i,j} - X_{i,k}(Y_{k,i}^T X_{k,j})Y_{k,j}^T$ 
10:    end for
11:  end for

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The  $\mathcal{O}(n^2)$  complexity of a standard, full rank solution of a 3D problem (of  $N$  unknowns) from the Laplacian operator discretized with a 3D 7-point stencil is reduced to  $\mathcal{O}(n^{5/3})$  when using the BLR format (Amestoy et al., 2015b). Although compression rates may not be as good as those achieved with hierarchical formats, BLR offers a good flexibility thanks to its simple, flat structure. This makes BLR easy to adapt to any multifrontal solver without a complete rethinking of the code.

Next, we describe the generalization of the BLR to a parallel environment. The row-wise partitioning imposed by the distribution of the front onto several processes constraints the clustering of the unknowns. However, in practice, we manage to maintain nearly the same compression rates when the number of processes grows (see Figure 3). Both LU and CB compression can contribute to reducing the volume of communication by a substantial factor and improving the parallel efficiency of the solver. In our implementation, we do not compress the CB. To fully exploit multicore architectures, MPI parallelism is hybridized with thread parallelism by multithreading the tasks of Algorithm 1. In full-rank, we exploit multithreaded BLAS kernels. In low-rank, these tasks have a finer granularity and thus a lower efficiency (flop rate). Thus with multithreaded BLAS we are not able to efficiently transform the compression of flops into reduction in time. To overcome this obstacle, Algorithm 1 can be modified to exploit OpenMP-based multithreading instead, which allows for a larger granularity of computations. The Update task at line 9 is applied on a set of independent blocks  $A_{i,j}$ : therefore, the loop at line 8 can be parallelized. The same applies for the Solve and Compress tasks: the loop at line 4 can also be parallelized using OpenMP.

## Seismic modeling with a Block Low-Rank direct solver

### NUMERICAL EXAMPLE

We perform finite-difference frequency-domain seismic modeling (Operto et al., 2014) in a visco-acoustic vertical transverse isotropic (VTI) subsurface model of the Valhall oil field (Barkved et al., 2010). This subsurface model, whose dimensions are  $16\text{km} \times 9\text{km} \times 4.5\text{km}$ , has been developed by reflection traveltime tomography (courtesy of BP) (Fig. 4a). We perform seismic modeling for the 5-Hz, 7-Hz and 10-Hz frequencies using 12, 16 and 34 computer nodes, respectively. Each node is made of two 10-core IvyBridge E5-2670v2 processor equipped with 64GB of shared memory. We ran 2 MPI processes per node and 10 threads per MPI process (i.e., 1 thread per core). The full-rank (FR) and the BLR factorizations are performed with single precision arithmetic. A discretization rule of 4-grid points per minimum wavelength leads to a grid interval of 70m, 50m and 35m and a finite-difference grid with perfectly-matched layers of 2.94, 7.17 and 17.27 millions of nodes for the three above-mentioned frequencies. The BLR solutions are computed for two values of the threshold  $\epsilon$  ( $10^{-4}$  and  $10^{-5}$ ).

### Computational efficiency and accuracy of BLR solver

The reduction of the memory demand, operation count and factorization time obtained with the BLR approximation are outlined in Table 1 for the three modeled frequencies. Compared to the FR factorization, the time to perform the BLR factorization ( $\epsilon = 10^{-5}$ ) is decreased by a factor 1.78, 2.15 and 2.87 for the 5Hz, 7Hz and 10Hz frequencies, respectively. This shows that the computational gain provided by the BLR approximation increases with frequencies (i.e., for larger matrices). The same trend is shown for the memory demand of the LU factorization.

The accuracy of the BLR solver is assessed by the differences between the FR solution and the BLR solutions for the 7-Hz frequency (Fig. 5). This difference is negligible for  $\epsilon = 10^{-5}$  and may be acceptable for FWI applications for  $\epsilon = 10^{-4}$  as shown hereafter. We apply FWI to a Valhall ocean-bottom cable dataset composed of 2302 hydrophone sensors and 49,954 shots using the FR and BLR solver with  $\epsilon$  equal to  $10^{-4}$  and  $10^{-5}$ . Eight frequencies between 3.5Hz and 7Hz are inverted successively (see Amestoy et al. (2015a) for more details). The final FWI models obtained with the FR and BLR ( $\epsilon = 10^{-4}$ ) solvers are very similar. Comparison between the 7-Hz recorded data and the synthetic data computed in the FWI model that has been built with the BLR solver shows an excellent agreement (Fig. 5(d-g)).

### Parallel performance and scalability of BLR solver

A parallel performance and strong scalability analysis of the FR and BLR solvers is performed in the Valhall model for the 7Hz frequency using 160, 320 and 640 cores (Fig. 3). The BLR version using multithread BLAS kernels does not fully exploit the compression potential: even though the flops are reduced by a factor 5.9, the time is only reduced by a factor 1.8. With OpenMP-based parallelism, we manage to retrieve a substantial part of this potential, reaching a speedup of 3.3. The scalability of FR solver is good: it obtains a speedup of 1.75 from 160 to 320 cores and of 1.4 from 320 to 640 cores.

The difference between the FR and BLR (with OpenMP) execution times decreases as the number of cores increases. This is due to the fact that the BLR code performs much less Flops and of much smaller granularity; nonetheless the strong scalability of the LR factorization is satisfactory and it is reasonable to expect that on problems of larger size, this difference remains considerable even on higher core counts, as evidenced by Table 1.

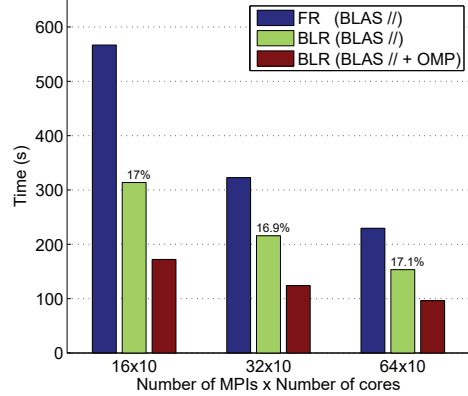


Figure 3: Scalability of the factorization for the 7Hz frequency. For BLR, the threshold has been set to  $\epsilon = 10^{-4}$ . *FR (BLAS //)*: Full-rank factorization. *BLR (BLAS //)*: BLR factorization using MKL BLAS kernels for multithreading. *BLR (BLAS // + OMP)*: BLR factorization using OpenMP for multithreading the Update and Compress tasks, MKL BLAS for the rest. The flop compression rate, provided on top of each bar, remains comparable when the number of processes grows.

## CONCLUSION

We have shown the computational efficiency, the accuracy and the parallel performance and scalability of the Block Low-Rank (BLR) algebraic sparse direct solver for frequency-domain seismic modeling. The computational time and memory savings achieved during BLR factorization increase with the size of the computational grid (i.e., frequency). This opens new perspectives to perform efficiently frequency-domain FWI of fixed-spread data on clusters of reasonable size at frequencies up to 15Hz. Other perspectives concern the optimization of the solution step, during which the sparsity of the source vectors can be exploited during the forward substitution step.

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## Seismic modeling with a Block Low-Rank direct solver

$f$	# cores	Flop count LU			Mem LU			Time LU		
		FR	BLR		FR	BLR		FR	BLR	
			$\epsilon = 10^{-5}$	$\epsilon = 10^{-4}$		$\epsilon = 10^{-5}$	$\epsilon = 10^{-4}$		$\epsilon = 10^{-5}$	$\epsilon = 10^{-4}$
5Hz	240	6.54E+13	26.5%	23.7%	2530 MB	53.4%	48.9%	80s	45s	40s
7Hz	320	4.05E+14	21.3%	16.9%	6445 MB	45.7%	39.1%	323s	150s	124s
10Hz	680	2.56E+15	20.3%	15.6%	10495 MB	42.5%	35.6%	1117s	389s	338s

Table 1: Statistics of the Full-Rank (FR) and Block Low-Rank (BLR) simulations for  $\epsilon = 10^{-5}$  and  $\epsilon = 10^{-4}$ .  $f$ : modeled frequency in Hertz. #cores: number of cores used; we ran 1 MPI process on each socket of 10 cores. Flop count: number of flops during LU factorization. Mem LU: Memory for LU factors in MegaBytes. Time LU: time for LU factorization in seconds. The flops and memory for the low-rank factorization are provided as percentage of those required by the full-rank factorization.

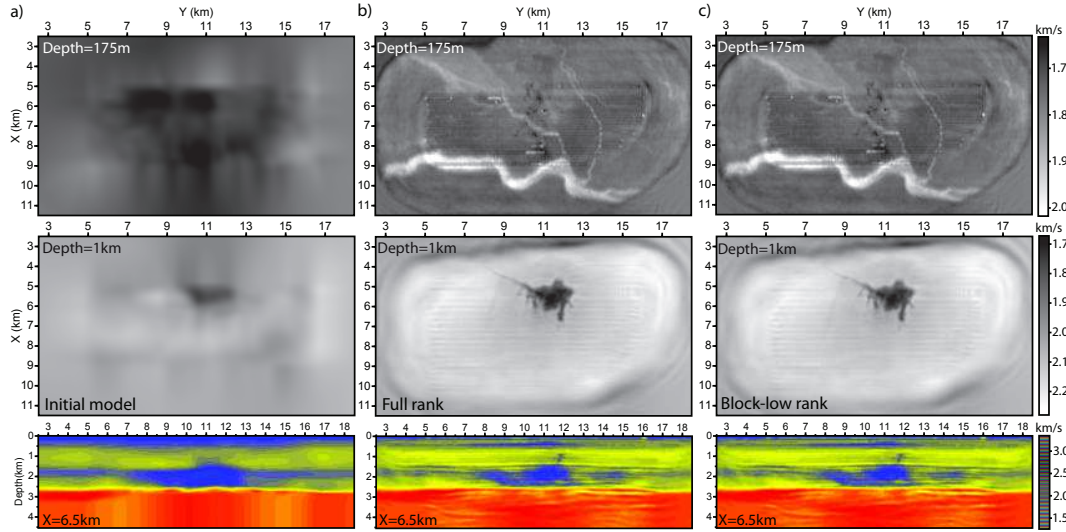


Figure 4: Traveltime tomography (a) and 7-Hz FWI (b-c) Valhall models. (b-c) FWI is performed with the FR (b) and the BLR( $\epsilon = 10^{-4}$ ) (c) solver. Top panel: horizontal slice across channel system; Middle panel: horizontal slice across a gas cloud; Bottom panel: vertical section near the periphery of the gas cloud ( $X=6.5\text{km}$ ) (see Sirgue et al. (2009) and Sirgue et al. (2010) for comparison).

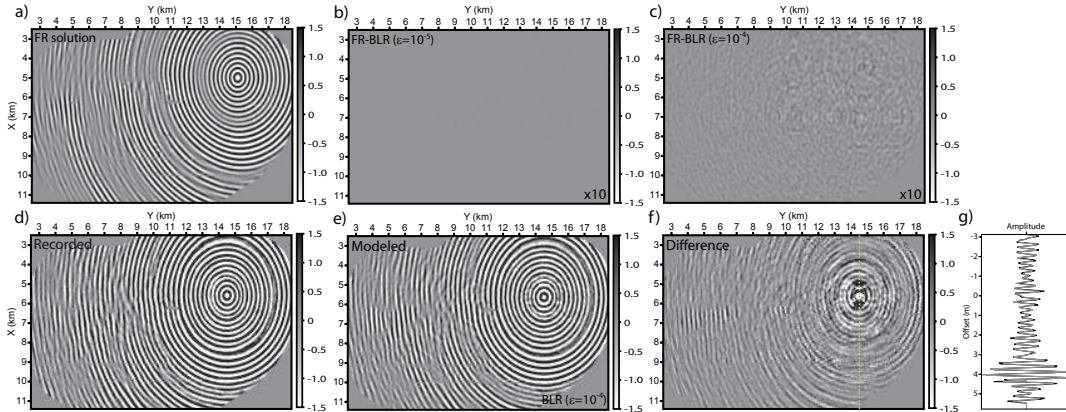


Figure 5: (a) 7-Hz FR solution (real part) computed in the tomography model (Fig. 4a). Pressure wavefield is shown at the shot positions, 5m below the surface. The explosive source,  $(X,Y)=(15\text{km},5\text{km})$ , is on the sea bottom at 70m depth. (b-c) Differences, magnified by a factor 10, between FR and BLR solutions ( $\epsilon = 10^{-5}$  (b),  $\epsilon = 10^{-4}$  (c)). (d) Recorded data (7Hz). (e) Synthetic data computed in the FWI model (Fig. 4c). (f) Residuals. (g) Comparison between (d, black) and (e, gray) along the yellow line.

## Seismic modeling with a Block Low-Rank direct solver

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