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Performance Analysis of SIMD vectorization of High-Order Finite-Element kernels.

Gauthier Sornet^(1,2), Sylvain Jubertie⁽¹⁾, Fabrice Dupros⁽²⁾, Florent De Martin⁽²⁾, Sebastien Limet⁽¹⁾
Univ. Orléans, INSA Centre Val de Loire, LIFO EA 4022.⁽¹⁾, BRGM, BP 6009, 45060 Orléans Cedex 2, France.⁽²⁾
Email: gauthier.sornet@univ-orleans.fr; sylvain.jubertie@univ-orleans.fr; f.dupros@brgm.fr;
f.demartin@brgm.fr; sebastien.limet@univ-orleans.fr

Abstract—Physics-based three-dimensional numerical simulations are becoming more predictive and are already essential for improving the understanding of natural phenomena, such as earthquakes, tsunamis, flooding or climate change and global warming. Among the numerical methods available to support these simulations, Finite-Element formulations have been implemented in several major software packages. The efficiency of these algorithms remains a challenge due to the irregular memory access that prevents to squeeze the maximum level of performance out of current architectures. This is particularly true at the shared-memory level with several levels of parallelism and complex memory hierarchies. Despite significant efforts, automatic optimizations provided by compilers and high-level frameworks are often far from the performances obtained from hand-tuned implementations. In this paper, we have extracted a kernel from the EFISPEC software package developed at BRGM (the French Geological Survey). This application implements a high-order finite-element method to solve the elastodynamic equation. We characterize the performance of the extracted mini-app considering key parameters such as the order of the approximation, the memory access pattern or the vector length. Based on this study, we detail specific optimizations and we discuss the results measured as regards to the roofline performance model on Intel Broadwell and Skylake architectures.

I. INTRODUCTION

The landscape of multicore processors or accelerators available to implement scientific applications leads to increasing concerns as regards to the real efficiency of key applications. Each vendor is working on next-generation hardwares able to overcome exascale barriers. These upcoming architectures will probably combine high number of heterogeneous computing cores associated with advanced memory technologies. Efforts to prepare applications for this upcoming system should rely on a deep understanding of the algorithms to predict the performances.

Finite-element methods are representative of such situation, as these numerical approaches lies at the heart of many open-source or commercial software packages. One of the key features of this class of algorithm is the ability to handle complex geometrical object shapes. On top of the complex and unstructured meshes generally involved, the algorithm implements irregular data access to match with both the local and the global computational phases. Moreover, the order of the interpolation

described by the basis functions significantly impacts the CPU-intensive element-by-element computational phase. Indeed, one common statement is that the increase of the order of approximation comes almost for free as regards to the improvement of the arithmetic intensity of the kernel.

Our effort in this paper is to conduct a comprehensive study of the performance of High-Order Finite-Element numerical kernels. In case of an explicit time-marching algorithm, the summation of the element contributions (assembly phase) is a bottleneck. Our study target a representative Finite-Element Method (FEM) application. EFISPEC code ([1]) is developed at BRGM, the French Geological Survey, and solves the three-dimensional elastodynamic equations. The standard version of this code is implemented in Fortran2003 and heavily relies on the MPI library. The kernel extracted corresponds to the computation of the internal forces and represents a maximum of 90% of the total elapsed time. This paper extends previous works dealing with mono-core vectorization [2] and data-layout reorganization [3]. Our contributions in this paper are as follows:

- Theoretical performance for FEM numerical kernels based on the roofline performance model [4].
- Study of the impact of the order of approximation as regards to the arithmetic intensity.
- Evaluation of both direct and indirect data access pattern on the peak performance.
- Comparison of the performance on Intel Broadwell and Skylake dual-socket computing nodes.

The paper proceeds as follows. Section II describes the related work. Section III details the elastodynamic equations and the spectral-element method implementation. Section IV details the challenges for efficient implementations on current architectures. In sections V and VI, we show the results obtained with AVX-2 and AVX-512 SIMD instructions. Finally, we conclude this study and present some future work.

II. RELATED WORK

Though this work of evaluating the performance of a finite-element numerical kernel has already been done by using simpler approaches (for instance the Mantevo bench-

mark¹, optimizing applicative performance is a continuous effort as regards to emerging chips (growing vectorization capabilities for instance).

Besides the scientific problems, one major challenge is to face key breakthroughs on both the hardware and software sides that will drive the community to the Exaflops. For instance, the energy consumption wall, for systems built with several millions of heterogeneous cores, remains an open topic. Consequently, both the scalability and the efficiency (computation and memory movements) of current applications are critical.

As regards to earthquakes modeling on distributed-memory systems, several references ([5], [6], [7]) underline the scalability of explicit formulations to solve the elastodynamic. In this case, we benefit from limited amount of point-to-point communications between neighboring MPI sub domains. Significant works have been made to extend this parallel results on heterogeneous and low-power processor ([8], [9]), mainly for the simpler Finite-Difference method. For example, both auto-tuning and machine learning strategies ([10], [11]) have been considered to explore the usual and large space of optimization parameters (compiler flags, space and time tiling, memory mapping). These approaches have not yet been fully investigated for High-Order Finite Element methods. This is probably due to the complexity of the implementation of such kernels.

Nevertheless, few papers discuss low levels parallelism for Finite-Elements based methods ([12], [13], [14], [15], [16]). Among these contributions, mesh coloring algorithms have gained significant attention these last few years due to their ability to reduce synchronizations at the shared-memory level. The counterpart is the limited efficiency as regards to cache memory. In [3] we have extended this approach to parallel FEM assembly on multi-core architectures by implementing colored packs of elements along with advanced vectorization strategies.

Finally, one can change the data structure as detailed in [2]. In this reference, the authors compared the SOA (Structure of Arrays) data layout to the AOS (Array of Structures). This strategy shows limited impact on the performances that are mainly governed by the efficiency at the SIMD level. If we exploit knowledge from the physics as regards to specific geometries (for instance in geosciences), we can benefit from hybrid approaches that combines a structured mesh (with regular data access for the main part of the computation) and unstructured meshes (with irregular data access). This approach has been successfully implemented in [17].

III. EFISPEC: SPECTRAL FINITE ELEMENT SOLVER

The spectral-element method (SEM) appeared more than 20 years ago in computational fluid mechanics [18], [19], [20]. The SEM is a specific formulation of the finite-

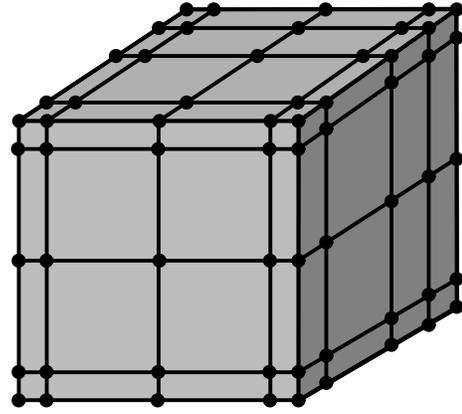


Figure 1: Referenced cube with $(4+1)^3 = 125$ GLL points.

A) Global GLL numbering						B) Local GLL numbering					
Element a			Element b			Element a			Element b		
1	2	3	3	10	13	a11	a12	a13	b11	b12	b13
4	5	6	6	11	14	a21	a22	a23	b21	b22	b23
7	8	9	9	12	15	a31	a32	a33	b31	b32	b33

Figure 2: Global and local view of the GLL numbering.

element method for which the interpolated points and the quadrature points of an element share the same location. These points are the Gauss–Lobatto–Legendre (GLL) points, which are the $p+1$ roots of $(1-\xi^2)P'_p(\xi) = 0$, where P'_p denotes the derivative of the Legendre polynomial of degree p and ξ coordinate in the one-dimensional reference space $\Lambda = [-1, 1]$.

The generalization to higher dimensions is done through the tensorization of the one-dimensional reference space. In three dimensions, the reference space is the cube $\square = \Lambda \times \Lambda \times \Lambda$ (see Fig. 1).

The mapping from the reference cubes to a hexahedral element Ω_e is done by a regular diffeomorphism $\mathcal{F}_e : \square \rightarrow \Omega_e$. In a finite-element method, the domain of study is discretized by subdividing its volume Ω into welded non-overlapping hexahedral elements Ω_e , $e = 1, \dots, n_e$ such that $\Omega = \cup_{e=1}^{n_e} \Omega_e$.

The elements Ω_e from the mesh of the domain. On the one hand, each element Ω_e has a local numbering of the GLL points ranging from 1 to $p+1$ along each dimension of the tensorization. On the other hand, the mesh has a unique global numbering ranging from 1 to N (see Fig. 2). The mapping from the local numbering to the global numbering is the so-called "assembly" phase of all finite-element calculations.

Each GLL point of an element Ω_e is redirected to a unique global number, $\forall \Omega_e$. When multiple elements share a common face, edge or corner, the assembly phase sums the local GLL value into the global numbering system.

¹<https://mantev.org/MantevOverview.pdf>

In this article, the problem of interest is the equation of motion whose weak formulation is given by

$$\int_{\Omega} \rho \mathbf{w}^T \cdot \ddot{\mathbf{u}} \, d\Omega = \int_{\Omega} \nabla \mathbf{w} : \boldsymbol{\tau} \, d\Omega - \int_{\Omega} \mathbf{w}^T \cdot \mathbf{f} \, d\Omega - \int_{\Gamma} \mathbf{w}^T \cdot \mathbf{T} \, d\Gamma$$

where Ω and Γ are the volume and the surface area of the domain under study, respectively; ρ is the material density; \mathbf{w} is the test vector; $\ddot{\mathbf{u}}$ is the second time-derivative of the displacement \mathbf{u} ; $\boldsymbol{\tau}$ is the stress tensor; \mathbf{f} is the body force vector and \mathbf{T} is the traction vector acting on Γ . Superscript T denotes the transpose, and a colon denotes the contracted tensor product.

Our study focuses on the internal forces defined by (see [21])

$$\begin{aligned} \int_{\Omega_e} \nabla \mathbf{w} : \boldsymbol{\tau} \, d\Omega_e \approx & \sum_{\alpha=1}^{p+1} \sum_{\beta=1}^{p+1} \sum_{\gamma=1}^{p+1} \sum_{i=1}^3 w_i^{\alpha\beta\gamma} \times \left[\right. \\ & \omega_{\beta} \omega_{\gamma} \sum_{\alpha'=1}^{p+1} \left[\omega_{\alpha'} \mathcal{J}_e^{\alpha'\beta\gamma} \sum_{j=1}^3 [\tau_{ij}^{\alpha'\beta\gamma} \partial_j \xi_{\alpha'}] \ell'_{\alpha}(\xi_{\alpha'}) \right] \\ & + \omega_{\alpha} \omega_{\gamma} \sum_{\beta'=1}^{p+1} \left[\omega_{\beta'} \mathcal{J}_e^{\alpha\beta'\gamma} \sum_{j=1}^3 [\tau_{ij}^{\alpha\beta'\gamma} \partial_j \eta_{\beta'}] \ell'_{\beta}(\eta_{\beta'}) \right] \\ & \left. + \omega_{\alpha} \omega_{\beta} \sum_{\gamma'=1}^{p+1} \left[\omega_{\gamma'} \mathcal{J}_e^{\alpha\beta\gamma'} \sum_{j=1}^3 [\tau_{ij}^{\alpha\beta\gamma'} \partial_j \zeta_{\gamma'}] \ell'_{\gamma}(\zeta_{\gamma'}) \right] \right] \end{aligned}$$

with $\boldsymbol{\tau}$ the stress tensor ($= \mathbf{c} : \nabla \mathbf{u}$); $\mathcal{J}_e^{\alpha'\beta\gamma}$ the jacobian of an element Ω_e at the GLL points $\alpha'\beta\gamma$; ω_{λ} integration weight at the GLL point λ ; ξ, η, ζ local coordinates along the three dimensions of the reference cube; ℓ'_{λ} derivative of the Lagrange polynomial at the GLL point λ . \mathbf{c} is the elastic tensor and $\nabla \mathbf{u}$ is the gradient of the displacement defined by

$$\begin{aligned} \partial_i u_j(\xi_{\alpha} \eta_{\beta} \zeta_{\gamma}) = & \left[\sum_{\sigma=1}^{p+1} u_j^{\sigma\beta\gamma} \ell'_{\sigma}(\xi_{\alpha}) \partial_i \xi_{\alpha\beta\gamma} \right] \\ & + \left[\sum_{\sigma=1}^{p+1} u_j^{\alpha\sigma\gamma} \ell'_{\sigma}(\eta_{\beta}) \partial_i \eta_{\alpha\beta\gamma} \right] \\ & + \left[\sum_{\sigma=1}^{p+1} u_j^{\alpha\beta\sigma} \ell'_{\sigma}(\zeta_{\gamma}) \partial_i \zeta_{\alpha\beta\gamma} \right] \end{aligned}$$

IV. CHALLENGES

A. Data access

The EFISPEC kernel has mainly to deal with unstructured meshes. Classical implementations require to use an indirection table. The elements are composed of GLLs identified by the numbers from this indirection table. This defined a GLL indirection table from the global GLL numbering to the local element GLL numbering.

For instance, the meshes of Geosciences can have some large computing zones with very local regions of interest. Moreover some unstructured sub-meshes can be located at the interfaces between two different regions represented by

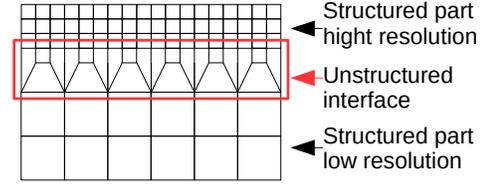


Figure 3: Mesh interface between two levels of resolution.

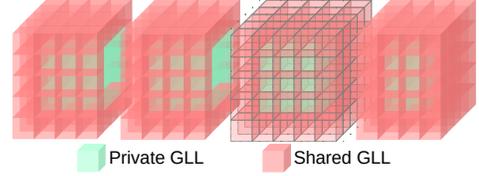


Figure 4: Gauss-Lobatto-Legendre (GLL) direct access structure

structures meshes a shown by the figure 3. Therefore, it was interesting to evaluate the performances of a regular access GLL structure as shown by the figure 4. It also allows the evaluation of the cost of the indirection involved in classical FEM assembly computations.

Structured meshes allow a direct data access structure that does not need to load any GLL indices. Therefore, the arithmetic intensity is higher. The elements can be organized following a three-dimensional grid as in the figure 3 .

B. Vectorization

The vectorization of our kernel is mainly described in the papers [3], [2]. It is based on the use of intrinsics since compilers are not able to fully vectorize the code. The principle is to compute elements eight by eight on AVX architectures or sixteen by sixteen on AVX-512 architectures. Mesh-partitioning procedures may rotate elements, thus the same GLL may be loaded several times in a SIMD register. In this case, scattering GLLs back to memory may cause concurrent writes. This problem is described in [2] and solved by adding a preprocessing step to detect and rotate elements to avoid this configuration. In our previous work, we have considered the AVX2 instruction set. In this paper, we also consider the AVX-512/256 instructions which are part of the AVX-512 instruction set but process only 256-bit of data. This brings scatter intrinsics to the AVX2 instruction set to implement the indirect data access algorithm. It allows to gather and scatter the GLL data between global and local numbering as shown in the figure 5. Thus, we can study the impact of doubling the SIMD width with the same instructions.

C. Arithmetic intensity

Each element of order o is composed of $(o + 1)^3$ GLLs. Computing an element consists of loading GLL values and executing floating point operations. Any loaded bytes can

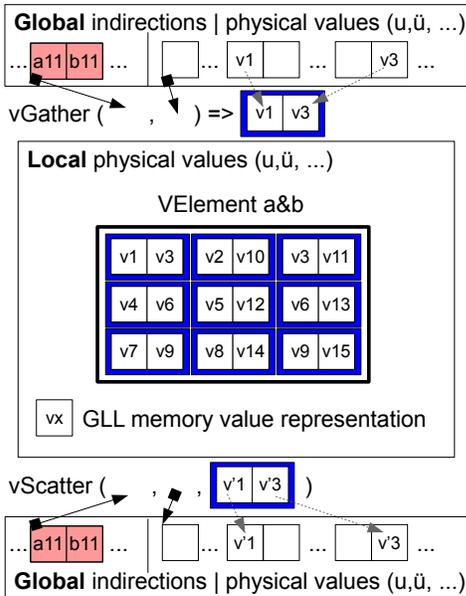


Figure 5: Description of the vectorization strategy.

be reused by the operations according to the element order as detailed in the table I.

To compute a 3 dimensional element of order 4 as one the figure 1, there are $(4 + 1)^3 = 125$ GLL values to load with other parameters (GLL weights or Lagrange derivatives). It costs 11120 bytes to load but 48150 floating point operations to compute. Then, the arithmetic intensity of an order 4 elements is $48150/11120 = 4.33$. This factor means that a byte is used for 4.33 flops. When the arithmetic intensity is low, we have to carefully optimize the memory access. Conversely, when it is high, we must pay attention to the computing capabilities. The AI threshold between computing and memory bandwidth bound depends on the architecture.

Order	Flop/Element	Data access	Byte/Element	A.I
2	7974	Regular	2316	3.44
		Irregular	2424	3.29
4	48150	Regular	10620	4.53
		Irregular	11120	4.33
8	411966	Regular	61596	6.69
		Irregular	64512	6.39

Table I: Arithmetic Intensity (A.I) with respect to the amount of data access and the order of the spectral element method. The irregular version uses an indirection array whereas the regular one uses a direct access to the physical values.

V. EXPERIMENTATIONS

A. Experimental setup

Two different platforms are considered. The first one is equipped with two Intel Xeon Gold 6148 processors based on the Skylake architecture. The second one comes with

Platform	Skylake	Broadwell
physical cores	2×20	2×18
base frequency	2.4GHz	2.3GHz
AVX frequency	1.9GHz	2.0GHz
AVX-512 frequency	1.6GHz	-

Table II: Platform characteristics

two Intel Xeon 2697v4 processors based on the previous Broadwell architecture. Table II contains the characteristics of both platforms. Hyperthreading is disabled on both platforms.

We propose to use the Roofline model to study the performance and the limitations of our implementations. The rooflines has been established for both platforms of results obtained from a BLAS SGEMM benchmark and the STREAM benchmark [22]. Figure 6 shows the resulting rooflines. The Broadwell and Skylake platforms achieve a peak performance of respectively 2,314 GFLOPS and 3,826 GFLOPS.

We consider two different compilers in our study: ICC 2017 and Clang 5. Since results obtained with neither compiler is significantly different and exhibit a similar behavior, we only present results obtained with Clang 5.

B. Kernels

We have derived several versions from the original EFISPEC kernel to study the impact of the approximation order and mesh structure. Two data access patterns are considered:

- 1) Irregular: the original EFISPEC access pattern based on an indirection array to access GLL elements in an unstructured mesh, also used in common FEM implementations.
- 2) Regular: GLL elements are stored in a regular pattern suitable to represent a structured mesh.

For each access pattern, we derive three variants for orders 2, 4 and 8. Each variant comes in three SIMD versions:

- 1) **AVX2**: it operates on 256-bit registers and is able to run on both the Broadwell and Skylake platforms,
- 2) **AVX-512**: it operates on 512-bit registers thus it is only able to run on the Skylake platform,
- 3) **AVX-512/256**: it is the same as the AVX2 version but uses a specific 256-bit SIMD scatter instruction (accessible through the `__mm256_i32scatter_ps` intrinsics) only available in the AVX-512 instruction set.

Comparing the AVX-512 and AVX-512/256 versions allows to study the gain brought by doubling the width of the SIMD unit. Note that, as reported in table II, cores adapt their frequency depending on the kind of SIMD instructions processed.

For each kernel, the corresponding arithmetic intensity, as indicated in table I, is reported into the rooflines. On both platforms, rooflines show that our kernels are memory-bound.

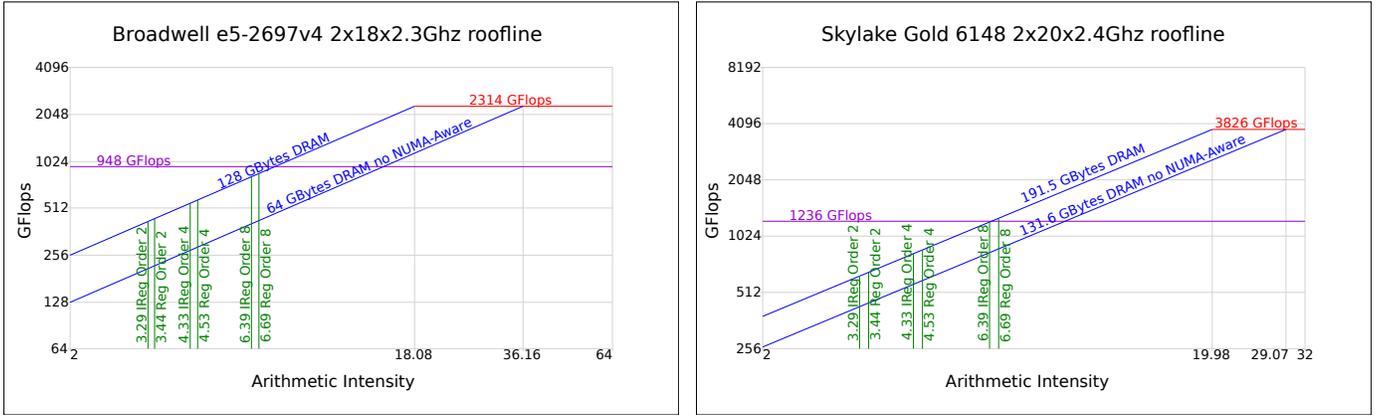


Figure 6: Rooflines for the Broadwell and Skylake platforms.

Additionally, we have introduced a peak application performance for each architecture. These values are computed with a small example able to fit into the cache. In this case we measure a peak value of 948 GFLOPS on Broadwell and 1,236 GFLOPS on Skylake. Based on these local peak performance, we can observe that the implementation of the order 8 versions are CPU-limited in almost all cases.

VI. EXPERIMENTAL RESULTS

A. Impact of the data access pattern

In this section, we comment on the impact of direct or indirect data access pattern on the performance observed. One of the key point is coming from the fact that an indirect data access implementation involves more data movement compared to a direct version (see Table I). In this case, each element requires to be transformed to a local representation before the compute and assembly phase. Even if the vectorization can deal with indirect loads and stores, we still need to retrieve the indices from DRAM to cache memory.

From figure 7, that represents the peak performance with respect to the data access strategy on Intel Broadwell and Skylake hardware, we can extract two main outcomes. First of all, the best results as regards to both scaling and peak performance are obtained with the direct and simpler data access pattern. This is expected as arithmetic intensities of these algorithms are higher (for instance the AI for the order 2 version is 3.44 in the direct case and 3.29 for the indirect case). Moreover these implementations can fully benefit from vectorization thanks to the regularity in the memory accesses.

Second of all, regardless of the polynomial order, the gap between direct and indirect data access versions is higher on Skylake. The direct data access pattern version outperforms the indirect one by 47% on Skylake but only by 34% on Broadwell for the higher polynomial order. Similar trend could be observed for lower polynomial orders as the benefit from regular data access pattern is clearly growing with the size of the SIMD vector.

B. Impact of the polynomial order

The main objective of this section is to discuss the impact of the order of approximation for the element-by-element computation. One common suggestion is that the extra computation coming with a higher polynomial order comes almost for free due to the arithmetic intensity improvement. This ideal scenario corresponds to a shift from a memory-bound to a CPU-bound situation.

If we study the shape of the plots from Broadwell and Skylake platforms (see Figure 7), we can observe a saturation of the peak performance as we increase the number of cores. This behavior could be explained by the roofline model and underlines that the higher order versions are more likely to be CPU-bound for direct access pattern. For irregular versions, the results on the Skylake platform are different as the lower order version performs better than the others. Similar trend could be observe on Broadwell hardware also with almost the same level of performance between both implementations.

These results do not match with the arithmetic intensity values (3.29 for order 2 and 6.39 at order 8). This is probably coming from a better usage of cache memory mainly for low order versions. In this case the local array is more likely to fit into the cache memory. When we increase the order of approximation, the amount of data is significantly larger, exceeding cache size and generating much more memory traffic at the DRAM level. To illustrate this, figure 8 compares local or remote memory access situations on our dual-socket shared-memory systems. If we compare both memory mapping strategies, the NUMA penalty leads to a revert ranking of the different implementations as regards to their peak performances.

C. Impact of the vectorization

The support of the AVX512 allows the hardware to compute 16 single precision floats by instruction. We recall from [3] that automatic optimizations provided by the

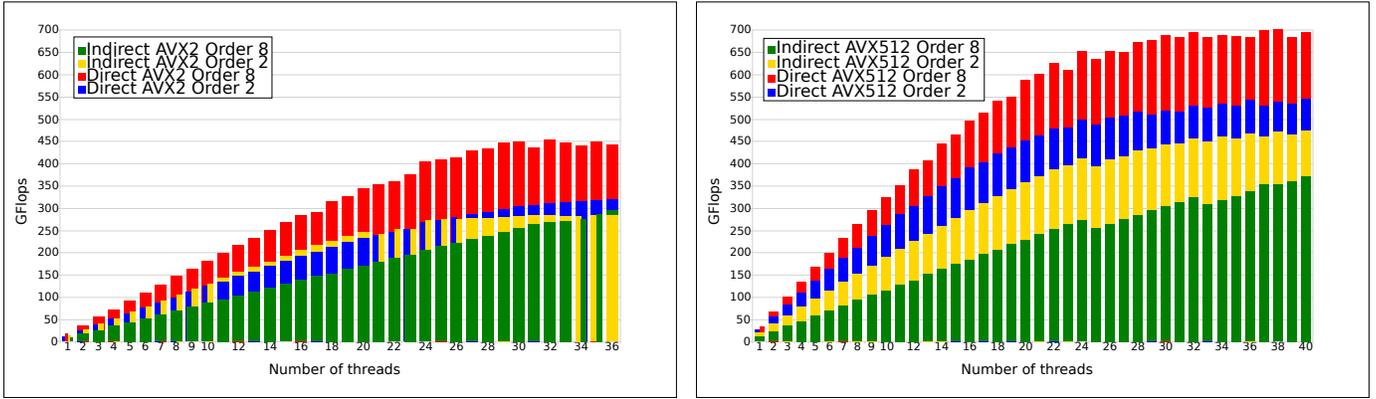


Figure 7: Comparison of the implementations with direct or indirect data access pattern on Broadwell (left) and Skylake (right) platforms.



Figure 8: Comparison of local or remote memory access strategies with the indirect data access pattern on Broadwell and Skylake platforms.

compilers hardly reach 140 GFLOPS on both platforms, this represents less than 5% of the theoretical peak performance. Figure 9 compares the performance between 256-bit and 512-bit SIMD instructions.

The AVX-512 with irregular data access version exhibits a speedup of 1.20 for order 2 and 1.13 for order 8 compared to AVX-512/256 implementations. As expected, the performance gain from the use of AVX-512 instructions is lower than 2 as regards to AVX-512/256. Conversely, the direct data access implementation benefits more from this improvement as we measure almost a speedup of 2.

D. Comparison with roofline model results

The arithmetic intensities of our different implementations are shown in Figure 6. Most of the kernels are bounded by the memory bandwidth. Therefore, we estimate the maximal GFLOPS peak performance of an implementation on a given platform by multiplying the peak memory bandwidth by the AI factor. For instance, the implementation based on an indirect data access pattern and an order 2 approximation (IReg Order 2) shows a peak performance of $3.29 \times 128 = 421.12$ GFLOPS.

The outcomes of the previous sections underline the fol-

lowing points. Firstly, the performance levels expected from the arithmetic intensity values are far from being reproduced during real experiments. For instance, the ratio between the AI for order 2 and order 8 implementations is 1.94. For simpler data access pattern and one core, measured results approximately match with the AI ratios (i.e. 1.51 on Broadwell and 1.21 on Skylake). When more computing cores are involved, the quality of the theoretical model tend to diminish due to a lack of refinement as regards to complex interactions at the shared-memory level.

Secondly, for the indirect memory access pattern, the ratio is reversed in almost all cases. That underlines the limitation of our model to take into account complex data movements on hierarchical architectures.

Data	AVX2	Order	1 thread	36 threads
Indirect access	/256	2	12.9 GFLOPS	284.1 GFLOPS
		8	8.6 GFLOPS	295.0 GFLOPS
Direct access	/256	2	11.9 GFLOPS	319.4 GFLOPS
		8	18.0 GFLOPS	442.3 GFLOPS

Table III: SIMD 256 bits performances from the Broadwell platform.

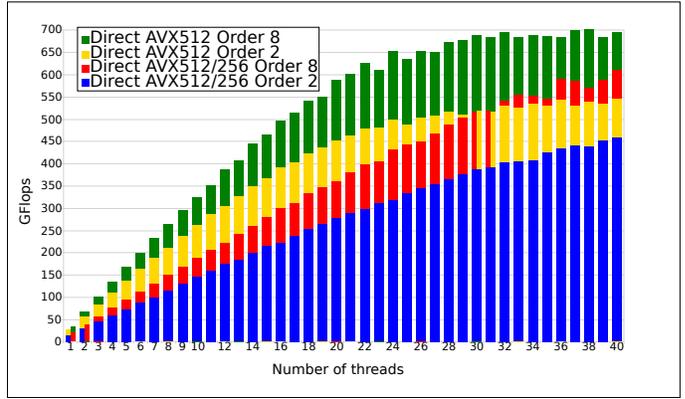
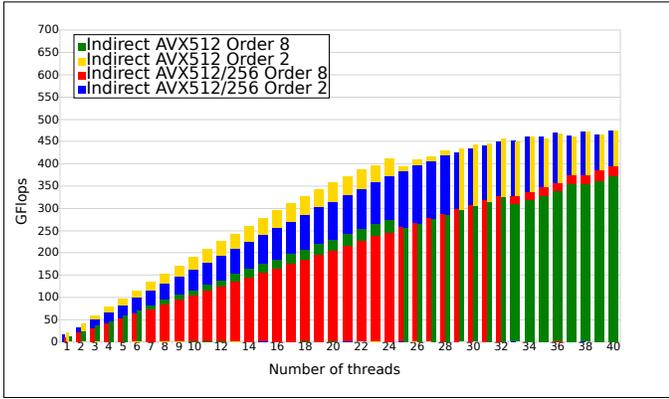


Figure 9: Comparison between AVX512 and AVX-512/256 with regular and irregular data access on the Skylake platform.

Data	AVX512	Order	1 thread	40 threads
Indirect access	/256	2	16.4 GFLOPS	474.0 GFLOPS
		8	10.4 GFLOPS	393.9 GFLOPS
	/512	2	19.6 GFLOPS	474.0 GFLOPS
		8	11.7 GFLOPS	371.2 GFLOPS
Direct access	/256	2	14.3 GFLOPS	458.4 GFLOPS
		8	19.1 GFLOPS	610.4 GFLOPS
	/512	2	28.2 GFLOPS	546.0 GFLOPS
		8	34.0 GFLOPS	696.0 GFLOPS

Table IV: SIMD 256 bits and SIMD 512 bits performances from the Skylake platform.

VII. CONCLUSION AND FUTURE WORK

Optimizing the most popular numerical methods for parallel architectures is a continuous effort. Though the main characteristics of these kernels are already well known, finding the best algorithms or implementations on each architecture can be viewed as a quest. Our paper underlines some of the key aspects of the Finite-Element Method by exploiting the popular roofline theoretical performance model. We also study the correlation between the arithmetic intensity and the real performance on two leading dual-socket Intel platforms.

Based on the theoretical model, we have underlined the impact of the data access patterns that represent a major bottleneck as regards to the expected performance. Additionally, from real experiments, we have demonstrated the limited improvements coming from higher polynomial orders on current architectures. One major outcome of this study is also the tremendous complexity of performance prediction, particularly on available chips that combine several levels of parallelism and cache hierarchies.

Obviously, the proposed optimizations would benefit from an integration in a high-level framework in order to ease their integration in a large number of scientific applications. We also believe that significant efforts should be made at the performance modeling level, probably with a wider usage of low-level emulation tools, to bring key applications up to speed on emerging processors.

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