COFFEE: an Optimizing Compiler for Finite Element Local Assembly

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***Abstract*—The finite element method is widely-employed to determine approximated solutions of partial differential equations. Local assembly is one of its fundamental steps, in which a suitable numerical procedure, or kernel, is applied to all elements in the discretized domain of the equation. Since the size of the domain can be huge, a notable problem consists of producing efficient kernels to minimize the cost local assembly. In this context, we present design, implementation and systematic performance evaluation of COFFEE, a domain-specific compiler for local assembly kernels. COFFEE manipulates kernels' abstract syntax trees by introducing composable optimizations aimed at improving instruction-level parallelism, especially in the form of SIMD vectorization, and register locality. It then generates C code, possibly including AVX or LRBNi intrinsics, which is eventually just-in-time compiled on the underlying architecture and executed. Performance evaluation using a suite of examples of real-world importance showed that speed-ups over non-optimized kernels between 1.32× and 4.44× can be achieved.**

Keywords*—*Finite element method, compilers, optimizations, simd vectorization

I. Introduction

In many fields, like computational fluid dynamics, computational electromagnetics, and structural mechanics, phenomena are modelled by means of partial differential equations (PDEs). Numerical techniques, like finite volume method and finite element method, are widely-employed to approximate solutions of PDEs. Unstructured meshes are often used to discretize the equation domain, since their geometric flexibility allows solvers to be extremely effective. The solution is sought in each cell of the discretized domain by applying suitable numerical kernels. As the number of cells can be of the order of millions, a major issue is the time required to execute the computation, which can be hours or days. To address this problem, domain-specific languages (DSLs) have been developed. The successful porting of Hydra, a computational fluid dynamics industrial application devised by Rolls Royce for turbomachinery design (based on Finite Volume Method, roughly 50000 lines of code and mesh sizes that can be over 100 millions edges), to OP2 [14], demonstrates the effectiveness of the DSL approach for implementing PDEs solvers [**?**].

OP2 adopts a kernel-oriented programming model, in which the computation semantics is expressed through self-contained functions, or "kernels". A kernel is applied to all elements in a set of mesh components (e.g. edges, vertices, cells/elements), with an implicit synchronization between the application of two consecutive kernels. On commodity multi-cores, a kernel is executed sequentially by a thread, while parallelism is achieved partitioning the mesh and assigning each partition to a thread. Similar programming and execution models are adopted in [13], [3], [5]. Kernel optimization is one of the major concerns in unstructured mesh applications. In this paper, we tackle this problem by proposing an optimization strategy for a class of kernels used in finite element methods.

We focus on local assembly ("assembly", in the following), a fundamental step of a finite element method that covers an important fraction of the overall computation run-time, often in the range 30%-60%. During the assembly phase, the solution of the PDE is approximated by executing a suitable kernel over all elements in the discretized domain. A kernel's working set is usually small enough to fit the L1 cache; it might need L2 cache when high-order methods are employed to improve the accuracy of the solution. However, we do not consider the latter case. An assembly kernel is characterized by the presence of an affine, often non-perfect loop nest, where individual loops are rather small (the trip count rarely exceeds 30, with a minimum value of 3, depending on the order of the method). With such small kernels, we focus on aspects like minimization of floating-point operations, register allocation and instruction-level parallelism, especially in the form of SIMD vectorization.

Optimization of assembly kernels is non-trivial. Given their structure and the exceptionally small size, assembly kernels benefit from transformations like generalized loop-invariant code motion, vector-register tiling and code splitting, which are not supported by state-of-the-art polyhedral and vendor compilers. BLAS routines could be theoretically employed, although fairly complicated control- and data-flow analysis would be required to automate identification and extraction of matrix-matrix multiplications. BLAS libraries are also known to perform far from peak performance when the dimension of the matrices is small [22]. As detailed in Section V, hand-made BLAS implementations of the Helmholtz assembly kernel (illustrated later) have run-times worse than those achieved with our optimization strategy.

Due to the constraints of available compilers and on linear-algebra specialized libraries, we have automated a set of generic and model-driven code transformations in COFFEE[1], a compiler for optimizing local assembly kernels. COFFEE is

[1]COFFEE stands for COmpiler For Finite ElemEnt local assembly.

```
Input: stiffness matrix A (initialized to 0),
       element coordinates in the domain (array),
       (optional) fields (e.g. velocity, array)
Output: stiffness matrix A (computed)
1  - Jacobian computation, using element coordinates
2  - Declaration of constant data, among which basis function
3  - Computation of the stiffness matrix
```

Fig. 1. General structure of a local assembly kernel generated by Firedrake.

integrated with Firedrake, a system for solving PDEs through the finite element method based on the OP2 abstraction [1]. It supports any problems expressible with this framework. This allows us to evaluate our code transformations in a range of real-world problems, varying key parameters that impact both solution accuracy and kernel cost, namely the polynomial order of the method (from $p = 1$ to $p = 4$) and the geometry of elements in the discretized domain (2D triangle, 3D tetrahedron, 3D prism).

Early experiments showed that Firedrake-generated code for non-trivial assembly kernels was sub-optimal. Our cost-model-driven sequence of source-to-source code transformations, aimed at improving SIMD vectorization and register data locality, can result in performance improvements up to 1.5× over "softly-optimized" code (i.e. where only basic transformations are performed, such as generalized loop-invariant code motion, padding, and data alignment), and up to 4.44× over original kernels. The contribution of this paper is threefold

- An optimisation strategy for a class of kernels widely-used in scientific applications, namely local assembly in the context of the finite element method. Our approach exploits domain knowledge to go beyond the limits of both vendor (e.g. *icc*) and research (e.g. polyhedral) compilers.
- Design and implementation of a compiler that automates the proposed code transformations for any problems expressible in Firedrake.
- Systematic evaluation using a suite of examples of real-world importance, and evidence of significant performance improvements.

The paper is organized as follows. In Section II we provide some background on local assembly, showing code generated by Firedrake and emphasizing critical computational aspects. Section III describes in detail the various code transformations, highlighting when and how domain-knowledge has been exploited. The design and implementation of our compiler is discussed in Section IV. Section V shows performance results. Related work are illustrated in Section VI, while Section VII concludes the paper.

II. Background

Local assembly consists of evaluating so called element stiffness matrix ("stiffness matrix", in the following) and element stiffness vector; in this work, we focus on computation of stiffness matrices, which is usually the costly part of the process. A stiffness matrix can be intuitively thought as an approximated representation of the PDE solution in a

```
1  void helmholtz(double A[3][3], double **coords) {
2    // K, det = Compute Jacobian (coords)
3
4    static const double W3[3] = {...}
5    static const double X_D10[3][3] = {{...}}
6    static const double X_D01[3][3] = {{...}}
7
8    for (int i = 0; i<3; i++)
9      for (int j = 0; j<3; j++)
10       for (int k = 0; k<3; k++)
11         A[j][k] += ((Y[i][k]*Y[i][j]+
12           +((K1*X_D10[i][k]+K3*X_D01[i][k])*
13           *(K1*X_D10[i][j]+K3*X_D01[i][j]))+
14           +((K0*X_D10[i][k]+K2*X_D01[i][k])*
15           *(K0*X_D10[i][j]+K2*X_D01[i][j])))*
16           *det*W3[i]);
17 }
```

Fig. 2. Local assembly code generated by Firedrake for a Helmholtz problem on a 2D triangular mesh with Lagrange $p = 1$ elements.

```
1  void burgers(double A[12][12], double **c, double **w) {
2    // K, det = Compute Jacobian (c)
3
4    static const double W5[5] = {...}
5    static const double X1_D001[5][12] = {{...}}
6    static const double X2_D001[5][12] = {{...}}
7    //11 other basis functions definitions.
8    ...
9
10   for (int i = 0; i<5; i++) {
11     double F0 = 0.0;
12     //10 other declarations (F1, F2,...)
13     ...
14     for (int r = 0; r<12; r++) {
15       F0 += (w[r][0]*X1_D100[i][r]);
16       //10 analogous statements (F1, F2, ...)
17     }
18     ...
19     for (int j = 0; j<12; j++)
20       for (int k = 0; k<12; k++)
21         A[j][k] += (..(K5*F9)+(K8*F10))*Y1[i][j])+
22          +(((K0*X1_D100[i][k])+(K3*X1_D010[i][k])+
23          +(K6*X1_D001[i][k]))*Y2[i][j]))*F11)+
24          +(..((K2*X2_D100[i][k])+...+(K8*X2_D001[i][k])*
25          *(K2*X2_D100[i][j])+...+(K8*X2_D001[i][j]))..)+
26          + <roughly a hundred sum/muls go here>)..)*
27          *det*W5[i]);
28   }
29 }
```

Fig. 3. Local assembly code generated by Firedrake for a Burgers problem on a 3D tetrahedral mesh with Lagrange $p = 1$ elements.

specific cell (or element) of the discretized domain. Numerical integration algorithms are widely-used in assembly codes to evaluate stiffness matrices [17], [3].

Given a mathematical description of the input problem, expressed through the domain-specific Unified Form Language [2], Firedrake generates C-code kernels implementing assembly using a numerical integration algorithm. It then triggers compilation of such kernels using an available vendor compiler, and eventually manages parallel execution over the mesh. The subject of this paper is to enhance this execution model by adding an optimization stage prior to the generation

of C code. The code transformations described next are also generalizable to non-Firedrake assembly kernels, provided that numerical integration is used.

The general structure of a Firedrake-generated kernel is shown in Figure 1. Input are a pointer to a 0-valued bi-dimensional array, which will be used to store the stiffness matrix; a pointer to the element's coordinates in the discretized domain; one or more pointers to so called fields, for instance indicating value of velocity or pressure in the element. The output is the evaluated element stiffness matrix. A local assembly kernel can be logically split into three parts: 1) calculation of the Jacobian matrix, its determinant and its inverse; 2) definition of some constant bi-dimensional arrays, called "basis functions" (or derivatives of basis functions) in finite element terminology, initialized to problem-specific double-precision floatin point values; 3) evaluation of the stiffness matrix in an affine loop nest. All elements in the discretized domain share the same basis function arrays, so they are declared as global read-only arrays (i.e. using `static const` in C language). Table I shows the variable names we will use in the upcoming code snippets to refer to the various kernel's objects.

Object name	Type	Variable name(s)
Determinant of Jacobian matrix	double	det
Inverse of Jacobian matrix	double[]	K
Coordinates	double**	coords
Fields	double**	w
Integration points	double[]	W
Basis functions (and derivatives)	double[][]	X, Y, X1, ...
Stiffness matrix	double[][]	A

TABLE I. TYPE AND VARIABLE NAMES USED IN THE VARIOUS CODE SNIPPETS TO IDENTIFY LOCAL ASSEMBLY OBJECTS.

The actual complexity of a local assembly kernel depends on the finite element problem being solved. In simpler cases, the loop nest is perfect, it has short trip counts (in the range 3-15), and the computation reduces to a summation of a few products. An example is provided in Figure 2, which shows an assembly kernel for a Helmholtz problem, using Lagrange basis functions on 2D elements with polynomial order $p = 1$. In other scenarios, for instance when solving a non-linear problem like Burgers as in Figure 3, the number of arrays involved in the computation of the stiffness matrix can be much larger: in this case, 14 unique arrays are accessed, and the same array can be referenced multiple times within the expression. Also, constants evaluated in outer loops (called F in the code), acting as scaling factors of arrays, may be required; trip counts can be larger (proportionally to the order of the method); arrays may be block-sparse. Note that in addition to a larger number of operations to compute the stiffness matrix, the Burgers case shows a register pressure higher than that in Helmholtz. Despite assembly kernels being problem-dependent, meaning that the space of codes that Firedrake can generate is infinite, it is still possible to identify common domain-specific traits, which can be exploited for effective code transformations and SIMD vectorization.

The class of kernels we are considering has, in particular, some peculiarities. 1) The computation of the Jacobian, which is the first step of the assembly, is independent of the loop nest. This is not true in general, since bent elements might be used in the unstructured mesh, which would require the Jacobian be re-computed at every i iteration; 2) memory accesses along the three loop dimensions are always stride-1; 3) the j and k loops are interchangeable, whereas permutation of i might be subjected to pre-computation of values (e.g. the F values in Burgers) and introduction of temporary arrays; 4) the j and k loops iterate over the same iteration space; 5) most of the sub-expressions on the right hand side of the stiffness matrix computation depend on just two loops (either i-j or i-k). In Section III we show how to exploit these observations to define a set of systematic, composable optimizations.

III. CODE TRANSFORMATIONS

The code transformations presented in this section are applicable to all finite element problems that can be formulated in Firedrake. One peculiar characteristic is that they all aim at improving the run-time of the `ijk` loop nest, where the numerical integration takes place. In rare, yet important cases, however, this might not be sufficient to achieve notable speed-ups. Generalized loop-invariant code motion, which is described in Section III-B, is a fundamental optimization that allows pre-computation of invariant sub-expressions. It is worth noting there are circumnstances in which the amount of lifted terms, either at the level of an outer loop or even completely outside of the loop nest, is so big (thousands of operations, hundreds of temporaries) that its execution time becomes the dominant factor of the overall local assembly run-time. In these cases, two challenging optimizations are common sub-expression elimination and effective vectorization (superword level parallelism [12] would not be of help, because invariant sub-expressions lack, in general, structure). Given its inherent complexity, a comprehensive study of this problem is left as further work.

A. Padding and Data Alignment

Auto-vectorization of assembly code computing the stiffness matrix can be less effective if data are not aligned and if the length of the innermost loop is smaller than the vector length vl. Data alignment is enforced in two steps. Initially, all arrays are allocated to addresses that are multiples of vl. Then, bi-dimensional arrays are padded by rounding the number of columns to the nearest multiple of vl. For instance, assume the original size of a basis function array is 3×3 and that the underlying machine possesses AVX, which implies $vl = 4$ since a vector register is 256 bits long and our kernels use 64-bits double-precision floating-point values. In this example, a padded version of the array will have size 3×4. The compiler is explicitly informed about data alignment using a suitable pragma. Padding of all bi-dimensional arrays involved in the evaluation of the stiffness matrix also allows us to safely round the loop trip count to the nearest multiple of vl. This avoids the introduction of a remainder (scalar) loop from the compiler, which would render vectorization less efficient.

B. Generalized Loop-invariant Code Motion

From inspection of the codes in Figures 2 and 3, it can be noticed that the computation of A involves evaluating many sub-expressions that depend on two iteration variables only. Since symbols in most of these sub-expressions are read-only variables, there is ample space for loop-invariant code motion. Vendor compilers apply this technique, although not in the systematic way we need for our assembly kernels. We

```
1  void helmholtz(double A[3][4], double **coords) {
2    #define ALIGN __attribute__((aligned(32)))
3    // K, det = Compute Jacobian (coords)
4
5    static const double W3[3] ALIGN = {...}
6    static const double X_D10[3][4] ALIGN = {{...}}
7    static const double X_D01[3][4] ALIGN = {{...}}
8
9    for (int i = 0; i<3; i++) {
10     double LI_0[4] ALIGN;
11     double LI_1[4] ALIGN;
12     for (int r = 0; r<4; r++) {
13       LI_0[r] = ((K1*X_D10[i][r])+(K3*X_D01[i][r]));
14       LI_1[r] = ((K0*X_D10[i][r])+(K2*X_D01[i][r]));
15     }
16     for (int j = 0; j<3; j++)
17       #pragma vector aligned
18       for (int k = 0; k<4; k++)
19         A[j][k] += (Y[i][k]*Y[i][j]+LI_0[k]*LI_0[j]+
20                     +LI_1[k]*LI_1[j])*det*W3[i]);
21   }
22 }
```

Fig. 4. Local assembly code generated by Firedrake when padding, data alignment, and *licm* are applied to the Helmholtz problem given in Figure 2. Data alignment and padding are for an AVX machine. In this specific case, sub-expressions invariant to j are identical to those invariant to k, so they can be precomputed once in a single loop r; in general, this might not be the case.

want to overcome two deficiencies that both *intel* and *gnu* compilers have. First, they can identify sub-expressions that are invariant with respect to the innermost loop only. This is an issue for sub-expressions depending on i-k, which are not automatically lifted in the default loop order `ijk`. Second, the hoisted code is scalar, i.e. it is not subjected to auto-vectorization. We work around these limitations with source-level loop-invariant code motion. In particular, we pre-compute all values that an invariant sub-expression assumes along its fastest varying dimension. This is implemented by introducing a temporary array per invariant sub-expression and by adding a new loop to the nest. At the price of extra memory for storing temporaries, the gain is that lifted terms can be auto-vectorized, because part of an inner loop. Given the short trip counts of our loops, it is important to achieve auto-vectorization of hoisted terms in order to minimize the percentage of scalar instructions, which could be otherwise significant. It is also worth noting that, in some problems, invariant sub-expressions along j are identical to those along k (e.g. in Helmholtz). In these cases, we safely avoid redundant pre-computation since, as anticipated in Section II, a property of our domain is that j and k loops share the same iteration space.

Figure 4 shows the Helmholtz assembly code after the application of loop-invariant code motion, padding, and data alignment.

C. Model-driven Vector-register Tiling

One notable problem of assembly kernels concerns register allocation and register locality. The critical situation occurs when loop trip counts and accessed variables are such that the vector-registers pressure is high. Since the kernel's working set fits the L1 cache, it is remarkably important to optimize register management. Canonical optimizations, such as loop interchange, unroll, and unroll-and-jam, can be employed to deal with this problem. In COFFEE, these optimizations are supported either by means of explicit code transformations (interchange, unroll-and-jam) or indirectly by delegation to the compiler through standard pragmas (unroll). Tiling at the level of vector registers is an additional feature of COFFEE. Based on the observation that the evaluation of the stiffness matrix can be reduced to a "summation of outer products" along the j and k dimensions, a model-driven vector-register tiling strategy can be implemented. If we consider the code snippet in Figure 4 (Helmholtz after loop-invariant code motion) and we ignore the presence of `det*W3[i]`, we can notice that the computation of the stiffness matrix is abstractly expressible as

$$A_{jk} = \sum_{\substack{x \in B' \subseteq B \\ y \in B'' \subseteq B}} x_j \cdot y_k \qquad j,k = 0,...,4 \tag{1}$$

where B is the set of all basis functions (or temporary variables, e.g. `LI_0`) accessed in the kernel, whereas B' and B'' are generic problem-dependent subsets. Regardless of the specific input problem, and by abstracting from the presence of all variables independent of both j and k, the stiffness matrix computation is always reducible to this kind of form. Figure 5 illustrates how we can evaluate 16 elements ($j,k = 0,...,4$) of the stiffness matrix using just 2 vector registers, which represent a 4×4 tile, assuming $|B'| = |B''| = 1$. Values in a register are shuffled each time a product is performed. Standard compiler auto-vectorization (*gnu* and *intel*), instead, executes 4 broadcast operations (i.e. "splat" of a value over all of the register locations) along the outer dimension to perform the calculation. Besides a larger number of cache accesses, it needs to keep between $f = 1$ and $f = 3$ extra registers to perform the same 16 evaluations when using unroll-and-jam, with f being the unroll-and-jam factor.

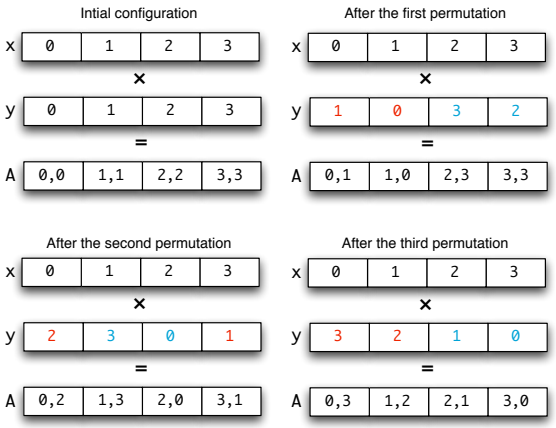

Fig. 5. Outer-product vectorization by permuting values in a vector register.

The storage layout of A, however, is incorrect after the application of this "outer-product vectorization" (*op-vect*, in the following). We efficiently restore it with a sequence of vector shuffles following the pattern highlighted in Figure 6, executed once outside of the `ijk` loop nest. The generated pseudo-code for the simple Helmholtz problem when using *op-vect* is shown in Figure 7.

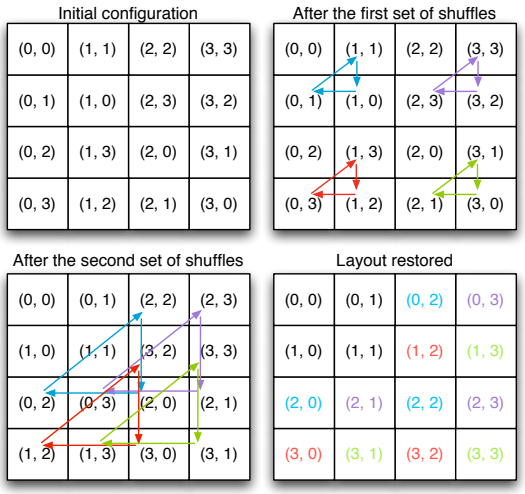

Fig. 6. Restoring the storage layout after *op-vect*. The figure shows how 4×4 elements in the top-left block of the stiffness matrix A can be moved to their correct positions. Each rotation, represented by a group of three same-colored arrows, is implemented by a single vector shuffle intrinsics.

D. Expression Splitting

In complex kernels, like Burgers' in Figure 3, and on certain architectures, achieving effective register allocation can be challenging. If the number of variables independent of the innermost-loop dimension is close to or greater than the number of available CPU registers, it is likely to obtain poor register reuse. This usually happens when the number of basis function arrays, temporaries introduced by generalized loop-invariant code motion, and problem constants is large. For example, applying loop-invariant code motion to Burgers on a 3D mesh needs 33 temporaries for the `ijk` loop order, and compiler's hoisting of invariant loads out of the k loop can be inefficient on architectures with a relatively low number of registers. One potential solution to this problem consists of suitably "splitting" the computation of the stiffness matrix A into multiple sub-expressions; an example, for the Helmholtz problem, is given in Figure 8. Splitting an expression has, in general, several drawbacks. Firstly, it increases the number of accesses to A proportially to the "split factor", which is the number of sub-expressions produced. Secondly, depending on how the split is executed, it can lead to redundant computation (e.g. the product $det * W3[i]$ is performed times number of sub-expressions in the code of Figure 8). Finally, it might affect register locality, although this is not the case of the Helmholtz example: for instance, the same array could be accessed in different sub-expressions, requiring a proportional number of loads be performed. Nevertheless, as shown in Section V, the performance gain from improved register reuse along inner dimensions can still be greater, especially if the split factor and the splitting itself use heuristics to minimize the aforementioned issues.

Table II summarizes the code transformations described so far. Given that many of these transformations depend on some parameters (e.g. tile size), we need a mechanism to prune such a large space of optimization. This aspect is treated in Section IV.

```
1  void helmholtz(double A[8][8], double **coords) {
2    // K, det = Compute Jacobian (coords)
3    // Declaration of basis function matrices
4
5    for (int i = 0; i<6; i++) {
6      // Do loop-invariant code motion
7      for (int j = 0; j<4; j+=4)
8        for (int k = 0; k<8; k+=4) {
9          // Call Load and set intrinsics
10         // Compute A[1,1],A[2,2],A[3,3],A[4,4]
11         // One permute_pd intrinsics per k-loop load
12         // Compute A[1,2],A[2,1],A[3,4],A[4,3]
13         // One permute2f128_pd intrinsics per k-loop load
14         // ...
15       }
16     // Do Remainder loop (from j = 4 to j = 6)
17   }
18   // Restore the storage layout:
19   for (int j = 0; j<4; j+=4) {
20     __m256d r0, r1, r2, r3, r4, r5, r6, r7;
21     for (int k = 0; k<8; k+=4) {
22       r0 = _mm256_load_pd (&A[j+0][k]);
23       // Load A[j+1][k], A[j+2][k], A[j+3][k]
24       r4 = _mm256_unpackhi_pd (r1, r0);
25       r5 = _mm256_unpacklo_pd (r0, r1);
26       r6 = _mm256_unpackhi_pd (r2, r3);
27       r7 = _mm256_unpacklo_pd (r3, r2);
28       r0 = _mm256_permute2f128_pd (r5, r7, 32);
29       r1 = _mm256_permute2f128_pd (r4, r6, 32);
30       r2 = _mm256_permute2f128_pd (r7, r5, 49);
31       r3 = _mm256_permute2f128_pd (r6, r4, 49);
32       _mm256_store_pd (&A[j+0][k], r0);
33       // Store A[j+1][k], A[j+2][k], A[j+3][k]
34     }
35   }
36 }
```

Fig. 7. Local assembly code generated by Firedrake when padding, data alignment, *licm* and *op-vect* are applied to the Helmholtz problem given in Figure 2. Here, we assume the polynomial order is $p = 2$, since *op-vect* can not be used when an iteration space dimension is smaller than the vector length. The original size of the j-k iteration space (i.e. before padding was applied) was 6×6. In this example, the unroll-and-jam factor is 1.

Name (Abbreviation)	Parameter
Generalized loop-invariant code motion (*licm*)	
Padding	
Data Alignment	
Loop interchange	loops
Loop unrolling	unroll factor
Register tiling	tile size
Outer-product vectorization (*op-vect*)	tile size
Assembly splitting (*split*)	split point, split factor

TABLE II. OVERVIEW OF CODE TRANSFORMATIONS FOR FIREDRAKE-GENERATED ASSEMBLY KERNELS.

IV. OVERVIEW OF COFFEE

Firedrake provides users with the Unified Form Language to write problems in a notation resembling mathematical equations. This high-level specification is translated by the Fenics Form Compiler [8] into an abstract syntax tree (AST) representation of one or more finite element assembly kernels. ASTs are then passed to COFFEE, which is capable of applying the transformations described in Section III. The output of COFFEE is C code, which is eventually provided

```
1  void helmholtz(double A[3][4], double **coords) {
2    #define ALIGN __attribute__((aligned(32)))
3    // K, det = Compute Jacobian (coords)
4    // Declaration of basis function matrices
5
6    for (int i = 0; i<3; i++) {
7      double LI_0[4] ALIGN;
8      double LI_1[4] ALIGN;
9      for (int r = 0; r<4; r++) {
10       LI_0[r] = ((K1*X_D10[i][r])+(K3*X_D01[i][r]));
11       LI_1[r] = ((K0*X_D10[i][r])+(K2*X_D01[i][r]));
12     }
13     for (int j = 0; j<3; j++)
14       #pragma vector aligned
15       for (int k = 0; k<4; k++)
16         A[j][k] += (Y[i][k]*Y[i][j]+LI_0[k]*LI_0[j])*det*W3[i];
17     for (int j = 0; j<3; j++)
18       #pragma vector aligned
19       for (int k = 0; k<4; k++)
20         A[j][k] += LI_1[k]*LI_1[j]*det*W3[i];
21   }
22 }
```

Fig. 8. Local assembly code generated by Firedrake when *split* is applied to the optimized Helmholtz problem given in Figure 4. In this example, the split factor is 2.

to PyOP2 [14], where just-in-time compilation and parallel execution over the unstructured mesh take place. Because of the large number of (possibly parametric) transformations, COFFEE needs a mechanism to select the most suitable optimization strategy for a given problem. Autotuning might be used, although at the moment we avoid it to minimize the run-time overhead. Our optimization strategy, based on heuristics and a simple cost model, is described in the following, along with an overview of the compiler.

The compiler structure is outlined in Figure 7. Initially, an AST is inspected, looking for the presence of iteration spaces and domain-specific information provided by the higher layer. If the kernel lacks an iteration space, then so-called inter-kernel vectorization, in which the non-affine loop over mesh elements is vectorized, can be applied. This feature, currently under development, has been proved to be useful in several Finite-Volume-based applications [20]. The second transformation step is applied if the backend is a manycore machine, like a GPU: the compiler tries to extract parallelism from inside the kernel, by partitioning loop iterations among different threads, if these are found to be independent [14]. Then, an ordered sequence of optimization steps are executed. Application of $licm$ must precede padding and data alignment, due to the introduction of temporary arrays. Based on a cost model, loop interchange, $split$, and $op\text{-}vect$ may be introduced. Their implementation is based on analysis and trasformation of the AST. When $op\text{-}vect$ is selected, the compiler outputs proper AVX (or LRBNi) intrinsics code. Any possible corner cases are handled: for example, if $op\text{-}vect$ is to be applied, but the size of the iteration space is not a multiple of the vector length, then a reminder loop, amenable to auto-vectorization, is inserted.

All loops are interchangeable provided that temporaries are introduced if the nest is not perfect. For the employed storage layout, the loop permutations `ijk` and `ikj` are likely

```
1  The COFFEE Compiler
   Input: ast, wrapper, isa
   Output: code
2  // Analyze ast and build optimization plan
3  it_space = analyze(ast)
4  if not it_space then
5      ast.apply_inter_kernel_vectorization(wrapper, isa)
       return wrapper + ast.from_ast_to_c()
6  endif
7  if isa.backend == gpu then
8      if it_space then
9          ast.extract_iteration_space(wrapper)
10     endif
11     return wrapper + ast.from_ast_to_c()
12 endif
13 plan = cost_model(it_space.n_inner_arrays, isa.n_regs)
14 // Optimize ast based on plan
15 ast.licm()
16 ast.padding()
17 ast.data_align()
18 if plan.permute then
19     ast.permute_assembly_loops()
20 endif
21 if plan.sz_split then
22     ast.split(plan.sz_split)
23 endif
24 if plan.uaj_factor then
25     uaj = MIN(plan.uaj_factor, ⌊it_space.j.size/isa.vf⌋)
26     ast.op_vect(uaj)
27 endif
28 return wrapper + ast.from_ast_to_c()
```

Fig. 9. Pseudocode of the COFFEE pipeline.

to maximize performance. Conceptually, this is motivated by the fact that if the i loop were in an inner position, then a significantly higher number of load instructions would be required every iteration; experiments showed that the performance loss is greater than the gain due to the possibility of accumulating increments in a register, rather than in memory, along the i loop. The choice between `ijk` and `ikj` depends on the number of load instructions that can be hoisted out of the innermost dimension. Our compiler chooses, as outer, the loop along which the number of invariant loads is smaller so that more registers are available to carry out the computation of the stiffness matrix.

Loop unroll and unroll-and-jam of outer loops are fundamental to expose instruction-level parallelism and register reuse, so tuning critical parameters, like the unroll factor, becomes of great importance. It is our experience (inspection of assembly code, comparison with other hand-made implementations), however, that for assembly kernels, where the loop nest is affine, bounds are usually very small and known at compile-time, and memory accesses are unit-stride, recent versions of a vendor compiler like $intel$'s employ cost models capable of estimating close-to-optimal values for such parameters. We leave therefore the backend compiler in charge to select the unroll factor. This choice also simplifies the COFFEE's cost model. The only situation in which we explicitly unroll-and-jam a loop is when $op\text{-}vect$ is used, since

```
1  Cost Model
   Input: n_outer_arrays, n_inner_arrays, n_consts, n_regs
   Output: uaj_factor, split_factor
2  n_outer_regs = n_regs / 2
3  split_factor = 0
4  // Compute spltting factor
5  while n_outer_arrays > n_outer_regs do
6      n_outer_arrays = n_outer_arrays / 2
7      split_factor = split_factor + 1
8  endw
9  // Compute unroll-and-jam factor for op-vect
10 n_regs_avail = n_regs - (n_outer_arrays + n_consts)
11 uaj_factor = ⌈n_reg_avail / n_inner_arrays⌉
12 if n_outer_arrays > n_inner_arrays then
13     permute = True
14 else
15     permute = False
16 endif
17 return <permute, split_factor, uaj_factor>
```

Fig. 10. The cost model is employed by the compiler to estimate the most suitable unroll-and-jam (when *op-vect* is used) and split factors, avoiding the overhead of auto-tuning.

the transformed code seems to prevent the $intel$ compiler from applying this optimization, even if specific pragmas are added. Note that, regardless of the output of the cost model, the unroll-and-jam factor never exceeds the actual size of the outer loop (line 25 in Figure 7, assuming the default loop order `ijk`).

The cost model is shown in Figure 8. It takes into account the number of available logical vector registers (n_regs) and the number of variables iterating along the j and k dimensions (n_consts for independent variables, n_outer_arrays for j variables, and n_inner_arrays for k variables, assuming the `ijk` loop order) to estimate unroll-and-jam and split factors when, respectively, $op\text{-}vect$ and $split$ are used. The n_consts parameter includes temporary registers to carry out computations, so setting its value is partly driven by heuristics. If a factor is 0, then the corresponding transformation is not applied. The $split$ transformation is triggered whenever the number of hoistable terms is larger than the available registers along the outer dimension (lines 3-8), which is approximated as half of the total (line 2). A split factor of n means that the assembly expression should be "cut" into n sub-expressions. Depending on the structure of the assembly expression, each sub-expression might end up accessing a different number of arrays; the cost model is simplified by assuming that all sub-expressions are of the same size. The unroll-and-jam factor for the $op\text{-}vect$ transformation is determined as a function of the available registers, i.e. those not used for storing hoisted terms (line 9-11). Finally, the profitability of loop interchange is evaluated (line 12-16)

V. Performance Evaluation

A. Experimental Setup

TODO: This section needs some rewording! And still lacks the Phi discussion!!

Experiments were run on two Intel machines, a Sandy Bridge (I7-2600 CPU, running at 3.4GHz, 32KB L1 cache and 256KB L2 cache) and the Phi. The `icc 13.1` compiler was used, with optimization level `-O2` and with auto-vectorization enabled (`-xAVX` on the Sandy Bridge, and `TODO` on the Phi). Other optimization levels performed, in general, slightly worse than `-O2`. Our code transformations were evaluated in three real-world problems based on the following PDEs:

- Helmholtz
- Advection-Diffusion
- Burgers

The code was written in UFL and then executed over real unstructured meshes through Firedrake. The Helmholtz code has already been shown in Figure 2. For Advection-Diffusion, the "Diffusion" equation, which uses the same differential operators as Helmholtz, is considered. In the Diffusion kernel, the main differences with respect to Helmholtz are the absence of the Y array and the presence of a few more constants for computing the stiffness matrix A. Burgers is a time-dependent problem, i.e. the assembly is recalculated every time step based on the result of previous iterations. It employs differential operators different from those of Helmholtz, which has a major impact on the generated assembly code (Figure 3), where a larger number of basis function matrices ($X1$, $X2$, ...) and constants ($F0$, $F1$, ..., $K0$, $K1$, ...) are accessed.

These problems were studied varying both the shape of mesh elements and the polynomial order p of the method. Intuitively, the bigger the element shape and p, the larger is the iteration space. Triangles (2D), tetrahedron (3D), and prisms (3D) were tested as element shape. For instance, in the case of Helmholtz with $p = 1$, the size of the j and k loops for the three kind of elements is, respectively, 3, 4, and 6. Moving from 2D to 3D has the effect of increasing the number of basis function arrays, since, conceptually, the behaviour of the equation has now to be approximated also along a third axis. On the other hand, the polynomial order affects only the problem size (the three loops i, j, and k, and, as a consequence, the size of X and Y arrays). A range of polynomial orders, from $p = 1$ to $p = 4$, were tested; higher polynomial orders are excluded from the study because of current Firedrake limitations. In such a large space of problems, the size of the stiffness matrix rarely excees 30×30, with a peak of 105×105 in Burgers with prisms and $p = 4$.

For the Helmholtz 3D problem, manual implementations based on `Intel MKL BLAS` were tested on the Sandy Bridge. This particular kernel can be easily reduced to a sequence of four matrix-matrix multiplies that can be computed via calls to BLAS `dgemm`. In the case of $p = 4$, where the stiffness matrix is of size 35×35, the computation was almost twice slower than the case in which only $licm$, data alignment and padding were used, with the slow down being even worse for smaller problem sizes. These experiments justify that there is a set of problems for which turning to MKL is not beneficial in terms of performance. It is possible that employing certain BLAS implementations or auto-tuning strategies for particular problem sizes is helpful, although the same problems afflicting $split$ (exposed in Section III-D) might limit the performance gain. However, as anticipated, extraction of matrix-matrix multiplies from analysis of the kernel's AST

and a strategy for their execution will be comprehensively addressed in further work.

B. Impact of Generalized Loop-invariant Code Motion

Table V-B illustrates the speed-ups obtained on the Sandy Bridge and the Phi machines when *licm*, data alignment, and padding are used, over non-transformed code. We distinguish between *licm* and *licm-ap*; the latter makes use of padding and data alignment. Inspection of assembly code generated by `icc` confirmed all limitations described in Section III-B: only sub-expressions invariant with respect to outer loops are hoisted and, interestingly, not vectorized. This motivates the usually significant gain obtained. Padding and data alignment enhance, in general, the quality of SIMD auto-vectorization. Sometimes the run-time of *licm-ap* is similar to that of *licm* because the stiffness matrix size is, without padding, already a multiple of the vector length, and data is automatically aligned. Occasionally *licm-ap* is slower than *licm* (e.g. in Burgers 3D p3). This is due to the large number of aligned temporaries introduced by *licm*, which probably induces cache associativity conflicts.

C. Impact of Vector-register Tiling

Figures 11 and 12 show the speed-ups achieved by applying *op-vect* on top of *licm-ap* to the Helmoltz and Diffusion kernels, respectively. For each problem instance we report two bars: one indicates the best run-time achieved by autotuning the unroll/unroll-and-jam factors, whereas the other shows the result retrieved by the COFFEE's cost model. In general, there is no substantial difference between the two. This is chiefly because assembly kernels fit the L1 cache, so estimating the run-time based on the quality of register allocation is relatively simple. The rationale behind these results is that, for smaller configurations, vector-register tiling is rarely helpful. This is due to the fact that in the considered problems the number of accessed arrays along the innermost loop dimension is rather small (between 2 and 4), so extensive unrolling is often enough to maximize register re-use when the loops are relatively short. On the other hand, as soon as the iteration space becomes too big, vector-register tiles are essential to minimize pipeline stalls. A maximum speed-up of 1.4× over *licm-ap* was observed in the Diffusion kernel when using a prismatic mesh and $p = 4$. Application of *op-vect* to the Burgers problem induces meaningful slow downs, because of the large number of arrays that, generally, need to be tiled. Expression splitting can be used in combination to *op-vect* to alleviate this issue; this is discussed in Section V-D.

D. Impact of Expression Splitting

Expression splitting, or loop fission, contributes to relieve register pressure. The transformation is useless if the stiffness matrix can be evaluated by accessing a relatively small number of basis functions (or temporary values introduced by *licm*), for which efficient register allocation can be already guaranteed. In the cases of Helmholtz and Diffusion, irrespective of split factor and cut, the only consequence of applying *split* is to augment the number of increments for evaluating the stiffness matrix. On the Sandy Bridge machine, slow downs up to 1.4× were observed in these two problems. The cost model, however, prevents the adoption of this transformation, since

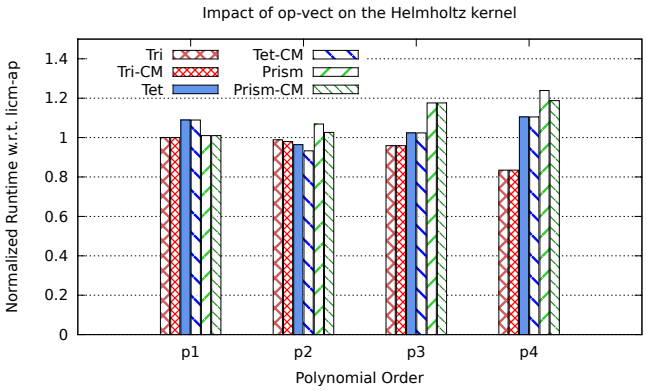

Fig. 11. Speed-ups obtained by applying *op-vect* on top of *licm-ap* to the Helmholtz kernel. Tri, Tet, and Prism stand, respectively, for triangual, tetrahedral and prismatic mesh. CM stands for cost model.

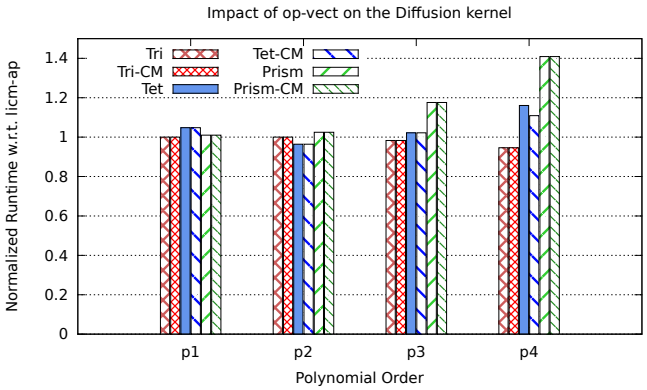

Fig. 12. Speed-ups obtained by applying *op-vect* on top of *licm-ap* to the Diffusion kernel. Tri, Tet, and Prism stand, respectively, for triangual, tetrahedral and prismatic mesh. CM stands for cost model.

the `while` statement at line 5 in Figure 8 is never entered. In the Burgers problem, *split* allows notable speed-ups to be achieved over the best run-time provided by either *licm* or *licm-ap*. Results are shown in Figure 13. In almost all problem configurations, a split factor of 1 induced optimal performance, meaning that the original expression was divided into two parts, with one part performing a slightly larger number of floating point operations than the other. Register locality could have been affected by requiring the same array be re-loaded twice as before splitting. However, in this experiment, this was only partly true, because most of the arrays appear in one sub-expression only.

VI. Related Work

The finite element method is used in the most disparate contexts to approximate solutions of PDEs. Well-known frameworks and applications include nek5000 [18], the Fenics project [13], Fluidity [3], and of course Firedrake; this is not an exhaustive list, though. Numerical integration is usually employed to implement the local assembly phase. The recent introduction of DSLs to decouple the finite element specification from its underlying implementation facilitated, however, the development of novel approaches. Methods based on tensor contraction [9] and symbolic manipulation [21] have been

		AVX		LRBNi	
		licm	licm+ap	licm	licm+ap
Helmholtz	tetrahedron	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×
Helmholtz	tetrahedron	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×
Helmholtz	prism	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×
Diffusion	triangle	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×
Diffusion	tetrahedron	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×
Diffusion	prism	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×
Burgers	triangle	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×
Burgers	tetrahedron	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×
Burgers	prism	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×	1.34×-4.32×

TABLE III. IMPACT OF GENERALIZED LOOP-INVARIANT CODE MOTION (*licm* COLUMN) ON THE HELMHOLTZ, DIFFUSION AND BURGERS PROBLEMS, FOR THREE KIND OF ELEMENTS BELONGING TO THE LAGRANGE FAMILY (TRIANGLE, TETRAHEDRON, PRISM), FOR THE RANGE OF POLYNOMIAL ORDERS $p \in \{1, 4\}$. EACH ENTRY INDICATES THE RANGE OF SPEED-UPS OBTAINED OVER THE NON-OPTIMIZED IMPLEMENTATION. THE COLUMN *licm-ap* ILLUSTRATES THE COMBINATION OF *licm* WITH DATA ALIGNMENT AND PADDING. RESULTS ARE SHOWN FOR BOTH THE SANDY BRIDGE AND THE PHI MACHINE.

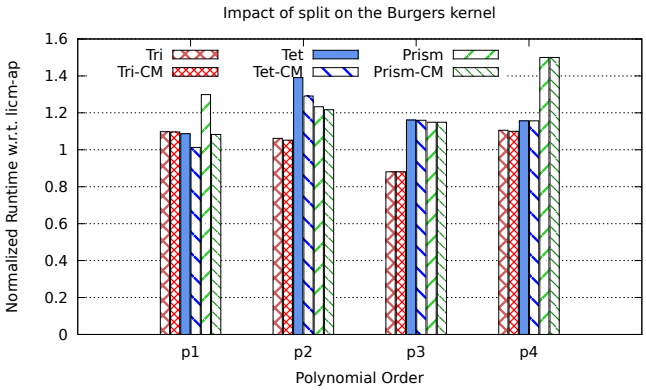

Fig. 13. Speed-ups obtained by applying *op-vect* on top of *licm-ap* to the Burgers kernel. Tri, Tet, and Prism stand, respectively, for triangular, tetrahedral and prismatic mesh. CM stands for cost model.

developed, although it has been demonstrated that numerical integration remains the optimal choice for a wide class of problems [17].

Optimization of local assembly using numerical integration for CPU platforms has been tackled in [17]. However, to the best of our knowledge, ours is the first work targeting low-level optimizations and adopting a real compiler approach. In [15], and more recently in [10], the problem has been studied for GPU architectures. In [11], variants of the standard numerical integration algorithm have been specialized for the PowerXCell processor and evaluated; The paper lacks, however, an exhaustive study from the compiler viewpoint as we did, and none of the optimizations presented in Section III are mentioned.

Domain-specific languages and automated code generation have been adopted with success in different areas. Spiral [19] automates generation of highly-optimized platform-specific digital signal processing numerical algorithms. Similar ideas are adopted in [23], where a DSL and a compiler for dense linear algebra kernels are proposed. OP2 [16], and its python implementation [14], which is used by Firedrake to express iteration over meshes, aim at achieving performance portability for scientific codes based on unstructured meshes. Stencil DSLs and compilers, such as Pochoir [25] and SDSL [7], have been developed to support development and high performance in fields like image processing and scientific computations over structured grids.

COFFEE currently uses a simple cost model and heuristics to steer the optimization process. Many code generators, like those based on the Polyhedral model [4] and those driven by domain-knowledge [24], make use of cost models. The other extreme consists of relying on auto-tuning to select the best implementation for a given problem on a certain platform. Notable examples include tuning of small matrix-matrix multiplies in nek5000 [22], the ATLAS library [26], and FFTW [6] for fast fourier transforms. In both cases, pruning the implementation space, as we did in Section IV, is fundamental to mitigate complexity and overhead.

VII. CONCLUSIONS

In this paper we have presented design, optimizations and systematic performance evaluation of COFFEE, a compiler for finite element local assembly. In this context, to the best of our knowledge, this is the first compiler oriented towards the introduction of low-level optimizations to maximize instruction-level parallelism, register locality and SIMD vectorization. Assembly kernels have peculiar characteristics. Their iteration space is usually very small, with the size depending on aspects like the degree of accuracy one wants to reach (polynomial order of the method) and the mesh discretization employed. The data space, in terms of number of matrices and scalar, grows proportionally to the complexity of the finite element problem. COFFEE has been developed taking into account all of these aspects, knowing that some transformations are useful only in a subset of all possible problems. The various optimizations overcome limitations of current vendor and research compilers. The exploitation of domain-knowledge allows some of them to be particularly effective, as demonstrated by our experiments on two state-of-the-art Intel platforms. Further work include a comprehensive study about feasibility and constraints of transforming the kernel into a sequence of BLAS calls. COFFEE supports all of the problems expressible in Firedrake, and it is already integrated with this framework.

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