

On Optimality of Finite Element Integration

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We tackle the problem of automatically generating optimal finite element integration routines given a high level specification of arbitrary multilinear forms. Optimality is defined in terms of floating point operations required to execute a loop nest. The generation of optimal loop nests is driven by a model that exploits mathematical properties of the domain of interest. A theoretical analysis and extensive experimentation prove the effectiveness of our approach, showing systematic performance improvements over a number of alternative code generation systems. The effect of low-level optimization is also discussed.

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1. INTRODUCTION

The need for rapidly implementing high performance, robust, and portable finite element methods has led to approaches based on automated code generation. This has been proved successful in the context of the FEniCS ([Logg et al. 2012]) and Firedrake ([Firedrake contributors 2014]) projects, which have become increasingly popular over the last years. In these frameworks, the weak variational form of a problem is expressed at high-level by means of a domain-specific language. The mathematical specification is manipulated by a form compiler that generates a representation of assembly operators. By applying these operators to an element in the discretized domain, a local matrix and a local vector, which represent the contributions of that element to the equation solution, are computed. The code for assembly operators should be high performance: as the complexity of a variational form increases, in terms of number of derivatives, pre-multiplying functions, or polynomial order of the chosen function

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spaces, the operation count increases, with the result that assembly often accounts for a significant fraction of the overall runtime.

As demonstrated by the considerable body of research on the topic, automating the generation of such high performance implementations poses several challenges. This is a result of the complexity inherent to the mathematical expressions involved in the numerical integration, which varies from problem to problem, and the particular structure of the loop nests enclosing the integrals. General-purpose compilers, such as *GNU's* and *Intel's*, fail at exploiting the structure inherent in the expressions, thus producing sub-optimal code (i.e., code which performs more floating-point operations, or “flops”, than necessary). Research compilers, for instance those based on polyhedral analysis of loop nests such as PLUTO ([Bondhugula et al. 2008]), focus on parallelization and loop optimization for cache locality, so they are not particularly helpful in our context. The lack of suitable third-party tools has led to the development of a number of domain-specific code transformation (or synthesizer) systems. In Olgaard and Wells [2010], it is shown how automated code generation can be leveraged to introduce optimizations that a user should not be expected to write “by hand”. In Kirby and Logg [2006] and Russell and Kelly [2013], mathematical reformulations of finite element integration are studied with the aim of minimizing the operation count. In Luporini et al. [2015], the effects and the interplay of generalized code motion and a set of low-level optimizations are analysed. It is also worth mentioning an on-going effort to produce a novel form compiler, called UFLACS ([Alnæs 2015]), which adds to the already abundant set of code transformation systems for assembly operators.

However, in spite of such a considerable research effort, still there is no answer to one fundamental question: can we automatically generate an implementation of a form which is optimal in the number of flops executed? In this paper, we formulate an approach to solve this problem. Summarizing, our contributions are as follows

- We characterize loop nest optimality and we instantiate this concept to finite element integration. As part of this construction, we establish the notion of sharing and demonstrate that sharing can always be eradicated from the loop nests we are interested in.
- We provide a model centred on sharing and other mathematical properties of our domain of interest; the model drives the translation of a monomial appearing in a form into optimal loop nests.
- We comment on the cases in which such model does not lead to optimal loop nests. We will see that this might occur with particular forms that make extensive use of tensor algebra. We show, however, that our model still is capable of producing quasi-optimal loop nests.
- We integrate the model with a compiler, COFFEE¹, which is in use in the Firedrake framework.
- We experimentally evaluate using a broader suite of forms, discretizations, and code generation systems than has been used in prior research. This is essential to demonstrate that our optimality model holds in practice.

In addition, in order to place COFFEE on the same level of other code generation systems from the viewpoint of low-level optimization (which is essential for a fair performance comparison)

- We introduce an engine based on symbolic execution that allows skipping irrelevant floating point operations (e.g., those involving zero-valued quantities). We elaborate

¹COFFEE stands for COMpiler For Fast Expression Evaluation. The compiler is open-source and available at <https://github.com/coneoproject/COFFEE>

on the performance impact of this optimization, making a clear distinction between flop optimality and efficient code.

2. PRELIMINARIES

We review finite element integration using the same notation and examples adopted in Olgaard and Wells [2010] and Russell and Kelly [2013].

We consider the weak formulation of a linear variational problem

$$\begin{aligned} &\text{Find } u \in U \text{ such that} \\ &a(u, v) = L(v), \forall v \in V \end{aligned} \quad (1)$$

where a and L are, respectively, a bilinear and a linear form. The set of *trial* functions U and the set of *test* functions V are discrete function spaces. For simplicity, we assume $U = V$. Let $\{\phi_i\}$ be the set of basis functions spanning U . The unknown solution u can be approximated as a linear combination of the basis functions $\{\phi_i\}$. From the solution of the following linear system it is possible to determine a set of coefficients to express u :

$$A\mathbf{u} = \mathbf{b} \quad (2)$$

in which A and \mathbf{b} discretize a and L respectively:

$$\begin{aligned} A_{ij} &= a(\phi_i(x), \phi_j(x)) \\ b_i &= L(\phi_i(x)) \end{aligned} \quad (3)$$

The matrix A and the vector \mathbf{b} are “assembled” and subsequently used to solve the linear system through (typically) an iterative method.

We focus on the assembly phase, which is often characterized as a two-step procedure: *local* and *global* assembly. Local assembly is the subject of this article. It consists of computing the contributions of a single element in the discretized domain to the equation solution. In global assembly, such local contributions are “coupled” by suitably inserting them into A and \mathbf{b} .

We illustrate local assembly in a concrete example, the evaluation of the local element matrix for a Laplacian operator. Consider the weighted Laplace equation

$$-\nabla \cdot (w \nabla u) = 0 \quad (4)$$

in which u is unknown, while w is prescribed. The bilinear form associated with the weak variational form of the equation is:

$$a(v, u) = \int_{\Omega} w \nabla v \cdot \nabla u \, dx \quad (5)$$

The domain Ω of the equation is partitioned into a set of cells (elements) T such that $\bigcup T = \Omega$ and $\bigcap T = \emptyset$. By defining $\{\phi_i^K\}$ as the set of local basis functions spanning U on the element K , we can express the local element matrix as

$$A_{ij}^K = \int_K w \nabla \phi_i^K \cdot \nabla \phi_j^K \, dx \quad (6)$$

The local element vector \mathbf{L} can be determined in an analogous way.

2.1. Quadrature Mode

Quadrature schemes are typically used to numerically evaluate A_{ij}^K . For convenience, a reference element K_0 and an affine mapping $F_K : K_0 \rightarrow K$ to any element $K \in T$ are introduced. This implies that a change of variables from reference coordinates X_0 to real coordinates $x = F_K(X_0)$ is necessary any time a new element is evaluated.

The numerical integration routine based on quadrature over an element K can be expressed as follows

$$A_{ij}^K = \sum_{q=1}^N \sum_{\alpha_3=1}^n \phi_{\alpha_3}(X^q) w_{\alpha_3} \sum_{\alpha_1=1}^d \sum_{\alpha_2=1}^d \sum_{\beta=1}^d \frac{\partial X_{\alpha_1}}{\partial x_{\beta}} \frac{\partial \phi_i^K(X^q)}{\partial X_{\alpha_1}} \frac{\partial X_{\alpha_2}}{\partial x_{\beta}} \frac{\partial \phi_j^K(X^q)}{\partial X_{\alpha_2}} \det F'_K W^q \quad (7)$$

where N is the number of integration points, W^q the quadrature weight at the integration point X^q , d is the dimension of Ω , n the number of degrees of freedom associated to the local basis functions, and \det the determinant of the Jacobian matrix used for the aforementioned change of coordinates.

2.2. Tensor Contraction Mode

Starting from Equation 7, exploiting linearity, associativity and distributivity of the involved mathematical operators, we can rewrite the expression as

$$A_{ij}^K = \sum_{\alpha_1=1}^d \sum_{\alpha_2=1}^d \sum_{\alpha_3=1}^n \det F'_K w_{\alpha_3} \sum_{\beta=1}^d \frac{X_{\alpha_1}}{\partial x_{\beta}} \frac{\partial X_{\alpha_2}}{\partial x_{\beta}} \int_{K_0} \phi_{\alpha_3} \frac{\partial \phi_i}{\partial X_{\alpha_1}} \frac{\partial \phi_j}{\partial X_{\alpha_2}} dX. \quad (8)$$

A generalization of this transformation has been proposed in [Kirby and Logg 2007]. By only involving reference element terms, the integral in the equation can be pre-evaluated and stored in temporary variables. The evaluation of the local tensor can then be abstracted as

$$A_{ij}^K = \sum_{\alpha} A_{i_1 i_2 \alpha}^0 G_K^{\alpha} \quad (9)$$

in which the pre-evaluated “reference tensor” $A_{i_1 i_2 \alpha}$ and the cell-dependent “geometry tensor” G_K^{α} are exposed.

2.3. Qualitative Comparison

Depending on form and discretization, the relative performance of the two modes, in terms of the operation count, can vary quite dramatically. The presence of derivatives or coefficient functions in the input form tends to increase the size of the geometry tensor, making the traditional quadrature mode preferable for “complex” forms. On the other hand, speed-ups from adopting tensor mode can be significant in a wide class of forms in which the geometry tensor remains “sufficiently small”. The discretization, particularly the relative polynomial order of trial, test, and coefficient functions, also plays a key role in the resulting operation count.

These two modes have been implemented in the FEniCS Form Compiler ([Kirby and Logg 2006]). In this compiler, a heuristic is used to choose the most suitable mode for a given form. It consists of analysing each monomial in the form, counting the number of derivatives and coefficient functions, and checking if this number is greater than a constant found empirically ([Logg et al. 2012]). We will later comment on the efficacy of this approach (Section 4. For the moment, we just recall that one of the goals of this research is to produce an intelligent system that goes beyond the dichotomy between quadrature and tensor modes. We will reason in terms of loop nests, code motion, and code pre-evaluation, searching the entire implementation space for an optimal synthesis.

3. PROBLEM CHARACTERIZATION

In this section, we characterize optimality for finite element integration and the loop transformation space that we need to explore to achieve it.

3.1. Loop Nests and Optimality

In order to make the document self-contained, we start with reviewing basic compiler terminology.

Definition 1 (Perfect and imperfect loop nests). *A perfect loop nest is a loop whose body either 1) comprises only a sequence of non-loop statements or 2) is itself a perfect loop nest. If this condition does not hold, a loop nest is said to be imperfect.*

Definition 2 (Independent basic block). *An independent basic block is a sequence of statements such that no data dependencies exist between statements in the block.*

We focus on perfect nests whose innermost loop body is an independent basic block. A straightforward property of this class is that hoisting invariant expressions from the innermost to any of the outer loops or the preheader (i.e., the block that precedes the entry point of the nest) is always safe, as long as any dependencies on loop indices are honored. We will make use of this property. The results of this section could also be generalized to larger classes of loop nests, in which basic block independence does not hold, although this would require refinements beyond the scope of this paper.

By mapping mathematical properties to the loop nest level, we introduce the concepts of a *linear loop* and, more generally, a (perfect) *multilinear loop nest*.

Definition 3 (Linear loop). *A loop L defining the iteration space I through the iteration variable i , or simply L_i , is linear if*

- (1) i appears in the body of L only as an array index, and
- (2) whenever an array a is indexed by i ($a[i]$), all expressions in which this appears are affine in a .

Definition 4 (Perfect multilinear loop nest). *A perfect multilinear loop nest of arity n is a perfect nest composed of n loops, in which all of the expressions appearing in the body of the innermost loop are linear in each loop L_i separately.*

Since our focus is on finite element integration, for simplicity we restrict ourselves to the following, notable subclass of perfect multilinear loop nests.

Definition 5 (Outer product loop nest). *An outer product loop nest is a perfect multilinear loop nest of arity $n \leq 2$ in which all of the expressions appearing in the body of the innermost loop are summations, and every loop index occurs in every summand.*

As shown later, outer product loop nests are important because they possess properties that we can take advantage of to synthesize optimal code. They arise naturally when translating bilinear or linear forms into code. Consider Equation 7 and the (abstract) loop nest implementing it illustrated in Figure 1. The imperfect nest $\Lambda = [L_e, L_i, L_j, L_k]$ comprises the element loop L_e , the integration loop L_i (a reduction loop), and the outer product loop nest $[L_j, L_k]$ over test and trial functions. The expression F implements the operator.

```

for (e = 0; e < L; e++)
  ...
  for (i = 0; i < M; i++)
    ...
    for (j = 0; j < N; j++)
      for (k = 0; k < O; k++)
        aejk += F(...)

```

Fig. 1: The typical loop nest implementing a bilinear form.

Our aim is a strategy to synthesize optimal loop nests of this form. In particular, we characterize optimality as follows.

Definition 6 (Optimality of a loop nest). *Let Λ be a generic loop nest, and let Γ be a generic transformation function $\Gamma : \Lambda \rightarrow \Lambda'$ such that Λ' is semantically equivalent to Λ (possibly, $\Lambda' = \Lambda$). We say that $\Lambda' = \Gamma(\Lambda)$ is an optimal synthesis of Λ if the number of operations that it performs to evaluate the result is minimal.*

Note that Definition 6 does not take into account memory requirements. If the loop nest were memory-bound – the ratio of operations to bytes transferred from memory to the CPU being too low – then speaking of optimality would clearly make no sense. Henceforth we assume to operate in a CPU-bound regime, in which arithmetic-intensive expressions need be evaluated. In the context of finite element, this is often true for more complex multilinear forms and/or higher order elements.

3.2. Transformation Space

To synthesize optimal implementations we need:

- a characterization of the space of legal loop transformations for the class of loop nests considered
- a cost model to select the optimal point in the transformation space

In this section, we construct the transformation space. We leave a few loose ends, which we progressively tie up in Section 4.

We start with introducing the fundamental notion of sharing.

Definition 7 (Sharing). *A loop L_i presents sharing if it contains at least one statement in which two (sub-)expressions depending on i are symbolically identical.*

Definition 8 (Sharing factor). *The sharing factor of a loop L_i , L_i^{sf} , is given by the cardinality of the set of symbols depending on i (i.e., arrays indexed by i). It provides an indication of the maximal number of symbols which can be factorized to the level of L_i .*

<pre> for (j = 0; j < 0; j++) for (i = 0; i < N; i++) a_{ji} += b_jc_i + b_jd_i </pre> <p style="text-align: center;">(a) With sharing</p>	<pre> for (i = 0; i < N; i++) t_i = c_i + d_i for (j = 0; j < 0; j++) a_{ji} += b_jt_i </pre> <p style="text-align: center;">(b) Optimal form</p>
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Fig. 2: A simple outer product loop nest. Note that $L_i^{sf} = 2$ and $L_j^{sf} = 1$.

Figure 2(a) shows an example of a trivial outer product loop nest of arity $n = 2$ with sharing along dimension j induced by b_j . Figure 2(b) shows an optimal synthesis for the loop nest in Figure 2(a). More in general, arbitrarily complex outer product loop nests can systematically be reduced to optimal form. The constructive proof that we provide below focuses on outer product loop nests of arity $n = 2$ (for $n < 2$ the proof is trivial; for $n > 2$, as we elaborate later, a more general treatise would be required).

Proposition 1. *Assume $\Lambda = [L_{i_0}, L_{i_1}]$ is an outer product loop nest with the body of L_{i_1} being an independent basic block. Then an optimal synthesis Λ' can be determined by eliminating sharing from both loops, starting from the loop with smallest sharing factor.*

Proof. The demonstration is by construction and exploits linearity. We start with “flattening” the expressions (e.g., by multiplication expansion) in the body of L_{i_1} ; this exposes the space of all possible factorizations. Since Λ is an outer product loop nest, the resulting expressions are summations of outer products.

We traverse the expression tree and determine the sharing factor of the two linear loops. We take the symbols depending on the loop with smallest sharing factor, L_i , and we incrementally factorize them. Due to linearity, each factored product P only has one symbol depending on L_i , and this symbol is now unique in the expression. The other term in P , independent of L_i , is, by definition, loop-invariant, and therefore hoisted such that redundant computation is avoided. We repeat the same process for the symbols along the loop with higher sharing factor, L_j . The transformations are semantically correct: multilinearity ensures deterministic factorization; perfectness ensures safeness of hoisting (see Luporini et al. [2015] for more details about generalized code motion).

We now have to demonstrate that the chosen factorization strategy, based on sharing factors, leads to optimality. This reduces to prove that the two following facts are true (we do it by contradiction).

- (1) Taking L_j , the loop with higher sharing factor, as point of departure would lead to a sub-optimal Λ' (optimal only in the best case). If we assumed this were false, there would be two possibilities to consider: A) both L_i and L_j present sharing over disjoint sets of outer products; B) at least one outer product induces sharing along both L_i and L_j . Case A) is quite trivial since there are no side effects in swapping the order of factorizations, so Λ' would actually be optimal (best case scenario). In case B), due to linearity, factorization produces a summation of L_j^{sf} outer products, as opposed to L_i^{sf} if we had started with L_i . However, note that factorization followed by hoisting is always a winning strategy: evaluation, at every iteration, of hoisted symbols requires one operation (a sum) instead of the two operations (a product and a sum) needed by an outer product. Since $L_j^{sf} > L_i^{sf}$, it is clear that Λ' could not be optimal, which contradicts the hypothesis.
- (2) Partial elimination of sharing would lead to a sub-optimal Λ' (optimal only in the best case). Let us assume, for a moment, that this is false. In this scenario, at least one symbol is excluded from the factored product. Without loss of generality, consider, for instance, $a_i(b_j + c_j + \dots) + a_i e_j + \dots$. It is fairly obvious to see that either there is another factorization opportunity along L_j (e_j is shared with some other terms), in which case no additional operations need be performed, or Λ' is sub-optimal. Consequently, the hypothesis is generally contradicted.

Note that if we were considering outer product loop nests of arity $n > 2$ we would need a much more complex construction to guarantee optimality. \square

We now observe that, for the larger class of finite element integration loop nests, the presence of sharing is a *sufficient but not necessary* condition for being in *non-optimal* form. Consider again the bilinear form implementation in Figure 1. We pose the following question: are we able to identify sub-expressions within F for which the reduction imposed by L_i can be pre-evaluated, thus obtaining a decrease in operation count proportional to the size of L_i , M ? The transformation we look for is exemplified in Figures 3(a) (input) and 3(b) (output); Figure 3(a) can be seen as a simple instance of the abstract loop nest in Figure 1.

Pre-evaluation opportunities can be exposed through an exploration of the expression tree transformation space. For arbitrary loop nests, this can be challenging. Further, the following issues arise when considering pre-evaluation opportunities:

```

for (e = 0; e < L; e++)
  for (i = 0; i < M; i++)
    for (k = 0; k < O; k++)
      aek += debikci + debikdi

```

(a) With reduction

```

for (i = 0; i < M; i++)
  for (k = 0; k < O; k++)
    tk += bik(ci + di)
for (e = 0; e < L; e++)
  for (k = 0; k < O; k++)
    aek = detk

```

(b) Pre-evaluated reduction

Fig. 3: Exposition (through factorization) and pre-evaluation of a reduction.

- as opposed to what happens with hoisting in outer product loop nests, the temporary variable size is proportional to the number of non-reduction loops crossed (for the bilinear form implementation in Figure 1, $N \cdot O$ for sub-expressions depending on $[L_i, L_j, L_k]$ and $L \cdot N \cdot O$ for those depending on $[L_e, L_i, L_j, L_k]$). This might shift the loop nest from a CPU-bound to a memory-bound regime, which might be counter-productive for actual runtime
- the transformations exposing pre-evaluation opportunities could increase the arithmetic complexity (e.g., expansion may increase the operation count; further examples will be provided later). This could overwhelm the gain inherent in pre-evaluation.

To summarize, so far we have highlighted four problems:

- (1) The need for an algorithm to expose pre-evaluation opportunities
- (2) Potential explosion in working set size
- (3) Potential increase in operation count due to manipulation of the expression tree
- (4) The need for a strategy to coordinate sharing elimination and pre-evaluation opportunities (sharing elimination could inhibit pre-evaluation; pre-evaluation might expose further sharing)

We expand on these points in Section 4. In order to address point 2, we conclude this section by providing a more refined definition of optimality.

Definition 9 (Optimality of a loop nest with bounded working set). *Let Λ be a generic loop nest, and let Γ be a generic transformation function $\Gamma : \Lambda \rightarrow \Lambda'$ such that Λ' is semantically equivalent to Λ (possibly, $\Lambda' = \Lambda$) and a set of memory constraints is satisfied. We say that $\Lambda' = \Gamma(\Lambda)$ is an optimal synthesis of Λ if the number of operations that it performs to evaluate the result is minimal.*

4. TRANSFORMATION ALGORITHM

In this section, we build a transformation algorithm capable of reducing finite element integration loop nests to optimal form. A fundamental aspect is the definition of a suitable cost function to assess the profitability of pre-evaluation (for which a deeper explanation will be provided). The optimality of the transformation algorithm is discussed.

4.1. Memory constraints

We will first consider two examples which motivate the need for memory constraints. Our point of departure is again the bilinear form implementation in Figure 1. Analogous considerations apply to forms of arbitrary arity.

The fact that $L \gg M, N, O$ suggests we should be cautious about hoisting mesh-dependent (i.e., L_e -dependent) expressions. Imagine Λ is enclosed in a time stepping loop. One could think of exposing (through some transformations) and hoisting any

time-invariant sub-expressions to minimize redundant computation at every time step. The working set size could then increase by a factor L . The gain in number of operations executed could therefore be overwhelmed, from a runtime viewpoint, by a much larger memory pressure.

A second, more general observation is that, for certain forms and discretizations, aggressive hoisting can make the working set exceed the size of some level of local memory (e.g. the last level of private cache on a conventional CPU, the shared memory on a GPU). For example, pre-evaluating geometry-independent expressions outside of Λ requires temporary arrays of size $N \cdot O$ for bilinear forms and of size N (or O) for linear forms. This can sometimes break such a “local memory threshold”. In our experiments (Section 6.2) we will carefully study this aspect.

Based on these considerations, we establish the following set of memory constraints:

- (1) the size of a temporary due to code motion cannot be larger than that of the outer product loop nest iteration space;
- (2) the total amount of memory occupied by the temporaries due to code motion cannot exceed a certain threshold, T_H .

A corollary of constraint 1) is that hoisting expressions involving geometry-dependent terms outside of Λ , which is a possibility we discussed at the beginning of this section, is now forbidden. This clearly shrinks the transformation space, pruning points that most likely would result in sub-optimal performance.

4.2. Reaching Optimality

We here discuss how we can systematically reach the goal set by Definition 9.

We reinforce the idea that eliminating sharing from the outer product loop nest does not suffice. As presaged in Section 3, we consider whether, and under what conditions, the reduction imposed by L_i could be pre-evaluated, thus reducing the operation count.

To partly answer this question, we make use of a result – the foundation of tensor contraction mode – from Kirby and Logg [2007]. Essentially, multilinear forms can be seen as sums of monomials, each monomial being an integral over the equation domain of products (of derivatives) of functions from discrete spaces; such monomials can always be reduced to a product of two tensors (see Section 2). We interpret this result at the loop nest level: with an input as in Figure 1, we can always dissect F into distinct sub-expressions (the monomials). Each sub-expression is factorizable so as to split constants from $[L_i, L_j, L_k]$ -dependent terms. These $[L_i, L_j, L_k]$ -dependent terms can be hoisted outside of Λ and stored into temporaries. As part of this process, the reduction induced by L_i is evaluated. Consequently, L_i disappears from Λ . This transformation is actually what we were referring to when we introduced pre-evaluation in Section 3.

Two issues should be addressed: understanding for which monomials pre-evaluation is profitable; coordinating pre-evaluation with sharing elimination, since the latter inhibits the former. In this section, we tackle the second issue, while we deal with the first one in Section 4.3. For this, we start with explaining the transformation algorithm, which pseudo-code is provided in Figure 4.

Our choice is to study the impact of pre-evaluation, as number of operations saved or introduced, “locally”; that is, for each monomial, “in isolation”. We then introduce the cost function $\theta : M \rightarrow \mathbb{Z}$, where M is the set of monomials in the form. $\theta(m)$ represents the change in operation count if pre-evaluation were applied to monomial m : a negative value indicates an increase, whereas a positive value indicates a gain. If pre-evaluation is found profitable (i.e., $\theta(m) > 0$), the sub-expression implementing m is extracted; the surrounding loop nest is suitably “cloned”; a sequence of transformation steps – involving expansion, factorization, and code motion – takes place (details in Section 5);

```

1 dissect the input expression into monomials
2 for each monomial  $m$ :
3   if  $\theta(m) > 0$  and memory constraints satisfied:
4     mark  $m$  as candidate for pre-evaluation
5 for each monomial  $m$ :
6   if  $m$  does not share terms with  $m'$ , an unmarked monomial:
7     extract  $m$  into a separate loop nest
8     apply pre-evaluation to  $m$ 
9 for each expression:
10  remove sharing

```

Fig. 4: High level view of the transformation algorithm

```

// Pre-evaluated tables
...
for (e = 0; e < L; e++)
  // Temporaries due to sharing elimination
  // (Sharing was a by-product of pre-evaluation)
  ...
  // Loop nest for pre-evaluated monomials
  for (j = 0; j < N; j++)
    for (k = 0; k < O; k++)
      A[e,j,k] += G'(...) + G''(...) + ...

  // Loop nest for monomials for which run-time
  // integration was found faster
  for (i = 0; i < M; i++)
    // Temporaries due to sharing elimination
    ...
    for (j = 0; j < N; j++)
      for (k = 0; k < O; k++)
        A[e,j,k] += H(...)

```

Fig. 5: The loop nest produced by the algorithm for an input as in Figure 1.

and, finally, the hoisted code is pre-evaluated using symbolic execution. The result is a set of n -dimensional tables (these can be seen as “slices” of the reference tensor at the math level), n being the arity of the multilinear form.

Because of symmetries in basis functions, pre-evaluation could produce identical tables. These are mapped to the same temporary. The transformed sub-expression (monomial) can therefore be characterized by the presence of sharing. This is why the last two lines of the algorithm, which goal is to eliminate sharing following the procedure described in Proposition 1, are transparently applied to all sub-expressions, regardless of whether pre-evaluation was used. The output of the transformation algorithm is as in Figure 5, assuming the usual input of Figure 1.

Note that due to the memory constraints imposed in the previous section, sharing elimination and pre-evaluation fully describe the transformation space in which the optimal is searched. We have defined them as high level operations on top of traditional expression-restructuring transformations such as code motion, re-association, and factorization. Other classes of loop transformations, for instance aimed at improving data locality or exposing parallelism, can obviously be neglected since they do not impact the operation count.

Finally, with Proposition 2, we elaborate on the optimality of this approach.

Proposition 2. *Consider an arbitrary multilinear form and the corresponding loop nest Λ implementing it. The form comprises a set of monomials, M . Let P be the set of pre-evaluated monomials, and let Z be the set of non pre-evaluated monomials (i.e., $Z = M \setminus P$). Assume that:*

- (1) *pre-evaluating different monomials does not result in identical tables;*
- (2) *there is no sharing of terms between monomials in P and monomials in Z .*

Then, the transformation algorithm produces an optimal Λ' as established by Definition 9.

Proof. We first comment on the assumptions. First, we notice that neither of them is a sufficient condition for non-optimality. In addition: 1) is inherently a pathological case, which we neglect; 2) might actually occur in forms with several monomials, although, in practice, this was never the case in none of the problems that we have investigated (which are more than those studied in this article). Therefore, we also neglect this scenario, which would otherwise require a “global analysis” of M .

The operation count for Λ' is $\Lambda'_{ops} = LNO(\Lambda'_{ops_1} + I\Lambda'_{ops_2})$ where Λ'_{ops_1} and Λ'_{ops_2} represent the operation counts for P and Z , respectively. L , M , N , and O are the trip counts of the corresponding loops.

We prove our claim by demonstrating the following: A) pre-evaluating any $Z_P : Z_P \subseteq Z$ would result in Λ''_{ops} such that $\Lambda''_{ops} > \Lambda'_{ops}$; B) not pre-evaluating any $P_Z : P_Z \subseteq P$ would result in Λ''_{ops} such that $\Lambda''_{ops} > \Lambda'_{ops}$.

A) By pre-evaluating the monomials in Z_P , we clearly have $\Lambda''_{ops_2} = \Lambda'_{ops_2} - I \cdot \delta$, where $\delta > 0$ is a parameter to indicate the reduction in operation count exhibited by the non pre-evaluated monomials. To prove A), we then need to convince ourselves that $\Lambda''_{ops_1} - I \cdot \delta \geq \Lambda'_{ops_1}$ holds. The only (corner) situation in which this might occur is whenever some of the pre-evaluated monomials in Z_P result in tables identical to those already deriving from P . If that were the case, more sharing elimination opportunities would be exposed, which in turn could break the optimality claim. Assumption 1) prevents this situation, so the statement is true.

B) Let us consider the non-trivial case: there are at least two monomials p and z that share terms, with $p \in P_Z$ and $z \in Z$. We have to consider the fact that there could be (practically rare) circumstances in which despite $\theta_{wo}(z) < \theta_w(z)$ and $\theta_w(p) < \theta_{wo}(p)$, we could have $\theta_{wo}^G(z, p) < \theta_w(p) + \theta_{wo}(z)$, where θ_{wo}^G is a hypothetical global oracle. The intuition behind this is that there could be a larger potential gain in sharing elimination that goes lost if monomials are inspected in isolation. An extreme example is a summation of mass matrices, in which each monomial is characterized by same test and trial functions, and by a different pre-multiplying coefficient (i.e., known) function. The previously discussed assumption 2) allows us to neglect this possibility, which then makes B) true. \square

4.3. Cost Function

It remains to tie up one loose end: the definition of the cost function θ . Since θ is expected to be used by a compiler to drive the transformation algorithm, requirements are simplicity and velocity.

We define $\theta(m) = \theta_{wo}(m) - \theta_w(m)$, where θ_{wo} and θ_w represent the operation counts for a monomial m without and with pre-evaluation, respectively. In the following, we explain how to derive these two values.

We can easily predict θ_{wo} thanks to our key property, linearity. This was explained in Proposition 1. A simple expression tree traversal suffices to obtain the cost of a

sharing-free outer product loop nest, namely Λ_{ops}^{ns} . Assuming I to be the size of L_i , we have that $\theta_{wo} = \Lambda_{ops}^{ns} \cdot I$.

Determining θ_w is more complicated. We first need to estimate the *increase factor*, ι , to account for the presence of (derivatives of) coefficients. This number captures the increase in arithmetic complexity due to the transformations enabling pre-evaluation. To contextualize, consider the example in Figure 6.

```

for (i = 0; i < M; i++)
  for (j = 0; j < N; j++)
    for (k = 0; k < O; k++)
      A[j,k] += B[i,j]*B[i,k]*(f[0]*B[i,0]+f[1]*B[i,1]+f[2]*B[i,2])

```

Fig. 6: Simplified loop nest for a pre-multiplied mass matrix.

One can think of this as the (simplified) loop nest originating from the local assembly of a pre-multiplied mass matrix. The sub-expression $f[0]*B[i,0]+f[1]*B[i,1]+f[2]*B[i,2]$ represents the field f over (tabulated) basis functions (array B). In order to apply pre-evaluation, the expression needs to be transformed to separate f from the integration-dependent (i.e., L_i -dependent) quantities. By expanding the products, we observe an increase in the number of $[L_j, L_k]$ -dependent terms of a factor 3 (the number of basis functions for f). Intuitively, ι captures the increase in non-hoistable operations due to the transformations that expose pre-evaluation opportunities.

With a single coefficient, as we just saw, ι directly descends from the cost of product expansion. In general, however, predicting ι is less straightforward. For example, consider the case in which a monomial has multiple coefficients over the same function space. Product expansion would now lead to identical sub-expressions that, as such, would be mapped to the same temporary once pre-evaluated. The resulting loop nest would then be characterized by sharing, with the actual operation count (i.e., once sharing elimination is applied) being smaller than that found with a more naive analysis. For a precise evaluation of ι , we need to calculate the k -combinations with repetitions of n elements, with k being the number of coefficient-dependent terms appearing in a product (in the example, there is only f , so $k = 1$) and n the cardinality of the set of symbols involved in the coefficient expansion (in the example, $B[i,0]$, $B[i,1]$, and $B[i,2]$, so $n = 3$; note that we are talking about sets here, so duplicates would be counted once).

If $\iota \geq I$ we can immediately say that pre-evaluation will not be profitable. This is indeed a necessary condition that, intuitively, tells us that if we add to the innermost loop more operations than we actually save from eliminating L_i , then for sure $\theta_{wo} < \theta_w$. This observation can speed up the compilation time by decreasing the analysis cost.

If, on the other hand, $\iota < I$, a further step is necessary to estimate θ_w . In particular, we need to calculate the number of terms ρ such that $\theta_w = \rho \cdot \iota$. Consider again Figure 6. In the case of the mass matrix, the body of L_k is simply characterized by the dot product of test and trial functions, $B[j]*B[k]$, so trivially $\rho = 1$. In general, ρ varies with the discretization and the differential operators used in the form. For example, in the case of the bilinear form originating from a standard bi-dimensional Poisson equation, the reader could verify that after a suitable factorization we would have $\rho = 3$. There are several ways of determining ρ . The fastest would be to extract it from high-level analysis of form and discretization; for convenience, in our implementation we have algorithms that, based on analysis of the expression tree, project the output of monomial expansion and factorization, which in turn gives us ρ .

5. CODE GENERATION

The transformation algorithm described in Section 4 has been implemented in COFFEE, the optimizer of finite element integration routines used in Firedrake. In this section, we describe several aspects related to code generation.

5.1. Automation through the COFFEE Language

COFFEE implements all optimizations by composing “building-block” transformations, which we refer to as “rewrite operators”. This has several advantages. Firstly, extendibility: novel transformations – for instance, sum-factorization in spectral methods – could be expressed using the existing operators, or with small effort building on what is already available. Secondly, generality: any sort of codes characterized by (linear, but also non-linear) loop nests with sharing can be optimized (obviously, without guarantees on optimality). In other words, COFFEE only exploits domain properties, and it is not specifically tied to finite element in any way. Thirdly, robustness: the same operators are exploited, and therefore stressed, by different optimization pipelines.

The rewrite operators, which implementation is based on abstract syntax tree manipulation, compose the COFFEE language. A non-exhaustive list of such operators includes expansion, factorization, re-association, generalized code motion. We have primarily used these operators to implement sharing elimination and pre-evaluation. Further, we have exploited them for heuristic optimization of the integration loop when this is non-linear (e.g., whenever the form has non-linear coefficients). In such a case, expansion, factorization, and code motion are applied greedily, selecting the term with highest sharing factor at each iteration, based on the observation that this should minimize sharing and promote hoisting.

5.2. Independence from Form Compilers

One of the key pillars of COFFEE is independence from form compilers. Being capable of handling generic abstract syntax trees, COFFEE can be leveraged by any suitably adapted form compiler. For example, in Firedrake a modified version of the FEniCS Form Compiler producing abstract syntax trees instead of strings is used. COFFEE itself provides an interface for building such abstract syntax trees. In particular, COFFEE aims to decouple the form manipulation (i.e., the “math level”) from code optimization (flops executed, low level optimization such as vectorization). Another viewpoint is: developers of form compilers should not worry about expression optimization in any way, since this is handled at a lower level.

To achieve this goal, COFFEE needs a strategy to minimize the execution of potentially “useless” flops due to simplistic implementations of non scalar-valued function spaces. For example, the most trivial quadrature mode in the FEniCS Form Compiler implements vector-valued function spaces by populating tabulated basis functions with blocks of zero-valued columns. For the local element matrix/vector evaluation, these blocks are iterated over in a single, rectangular iteration space. This preserves the semantics of the computation while keeping the implementation complexity extremely low, although it also introduces unnecessary operations (e.g., zero-valued summands due to multiplications by zero). COFFEE achieves full independence from form compilers (and so relieves the implementation burden) by providing a transformation to avoid the execution of such useless flops. A challenge for this transformation is restructuring the iteration spaces while preserving the effectiveness of low level optimizations, especially (auto-)vectorization.

Consider a set of tabulated basis functions with quadrature points along rows and functions along columns. For example, $A[i, j]$ provides the value of the j -th basis function at quadrature point i . In Olgaard and Wells [2010], a technique to avoid

iteration over zero-valued columns based on the use of indirection arrays (e.g. $A[B[i]]$, in which A is a tabulated basis function and B a map from loop iterations to non-zero columns in A) was proposed. Our approach aims to avoid such indirection arrays in the generated code. This is because we want to avoid non-contiguous memory loads and stores, which can nullify the benefits of vectorization.

The idea is that if the dimension along which vectorization is performed (typically the innermost) has a contiguous slice of zeros, but that slice is smaller than the vector length, then we do nothing (i.e., the loop nest is not transformed). Otherwise, we restructure the iteration space. This has several non-trivial implications. The most notable one is memory offsetting (e.g., $A[i+m, j+n]$), which dramatically enters in conflict with padding and data alignment. We use heuristics to retain the positive effects of both and to ensure correctness. Details are, however, beyond the scope of this paper.

The implementation is based on symbolic execution: the loop nests are traversed and for each statement encountered the location of zeros in each of the involved symbols is tracked. Arithmetic operators have a different impact on tracking. For example, multiplication requires computing the set intersection of the zero-valued slices (for each loop dimension), whereas addition requires computing the set union.

6. PERFORMANCE EVALUATION

6.1. Experimental Setup

Experiments were run on a single core of an Intel I7-2600 (Sandy Bridge) CPU, running at 3.4GHz, 32KB L1 cache (private), 256KB L2 cache (private) and 8MB L3 cache (shared). The Intel Turbo Boost and Intel Speed Step technologies were disabled. The Intel icc 15.2 compiler was used. The compilation flags used were `-O3`, `-xHost`, `-ip`.

We analyze the runtime performance of four real-world bilinear forms of increasing complexity, which comprise the differential operators that are most common in finite element methods. In particular, we study the mass matrix (“Mass”) and the bilinear forms arising in a Helmholtz equation (“Helmholtz”), in an elastic model (“Elasticity”), and in a hyperelastic model (“Hyperelasticity”). The complete specification of these forms is made publicly available².

We evaluate the speed-ups achieved by a wide variety of transformation systems over the “original” code produced by the FEniCS Form Compiler (i.e., no optimizations applied). We analyze the following transformation systems

- FEniCS Form Compiler: optimized quadrature mode (work presented in Olgaard and Wells [2010]). Referred to as `quad`
- FEniCS Form Compiler: tensor mode (work presented in Kirby and Logg [2006]). Referred to as `tens`
- FEniCS Form Compiler: automatic mode (choice between `tens` and `quad` driven by heuristic, detailed in Logg et al. [2012] and summarized in Section 2.3). Referred to as `auto`
- UFLACS: a novel back-end for the FEniCS Form Compiler (whose primary goals are improved code generation time and runtime). Referred to as `ufls`
- COFFEE: generalized loop-invariant code motion (work presented in Luporini et al. [2015]). Referred to as `cf01`
- COFFEE: optimal loop nest synthesis plus symbolic execution for zero-elimination (work of this article). Referred to as `cf02`

The values that we report are the average of three runs with “warm cache” (no code generation time, no compilation time). They include the cost of local assembly as well

²https://github.com/firedrakeproject/firedrake-bench/blob/experiments/forms/firedrake_forms.py

as the cost of matrix insertion. However, the unstructured mesh used for the simulations (details below) was chosen small enough to fit the L3 cache of the CPU so as to minimize the “noise” due to operations outside of the element matrix evaluation.

For a fair comparison, small patches (publicly available) were written to run *all* simulations through Firedrake. This means the costs of matrix insertion and mesh iteration are identical in all variants. Our patches make UFLACS and the FEniCS Form Compiler’s optimization systems generate code suitable for Firedrake, which employs a data storage layout different than that of FEniCS (e.g., array of pointers instead of pointer to pointers).

In Section 4.1, we discussed the importance of memory constraints. We then define T_H as the maximum amount of space that temporaries due to code motion can take. We set $T_H = L2_{size}$, that is, the size of the processor L2 cache (the last level of private cache). We recall that exceeding this threshold prevents the application of pre-evaluation. In our experiments, this happened in some circumstances. In such cases, experiments were repeated with $T_H = L3_{size}$ to verify the hypotheses made in Section 4.1. We later elaborate on this.

Following the methodology adopted in Olgaard and Wells [2010], we vary the following parameters:

- the polynomial order of test, trial, and coefficient (or “pre-multiplying”) functions, $q \in \{1, 2, 3, 4\}$
- the number of coefficient functions $nf \in \{0, 1, 2, 3\}$

While constants of our study are

- the space of test, trial, and coefficient functions: Lagrange
- the mesh: tetrahedral with a total of 4374 elements
- exact numerical quadrature (we employ the same scheme used in Olgaard and Wells [2010], based on the Gauss-Legendre-Jacobi rule)

6.2. Performance Results

We report the results of our experiments in Figures 7, 8, 9, and 10 as three-dimensional plots. The axes represent q , nf , and code transformation system. We show one subplot for each problem instance $\langle form, nf, q \rangle$, with the code transformation system varying within each subplot. The best variant for each problem instance is given by the tallest bar, which indicates the maximum speed-up over non-transformed code. We note that if a bar or a subplot are missing, then the form compiler failed at generating code because of either exceeding the system memory limit or unable to handle the form.

The rest of the section is structured as follows: we provide insights about the main message of the experimentation; we comment on the impact of autovectorization; we explain in detail, individually for each form, the performance results obtained.

High level view. The main observation is that our transformation strategy does not always guarantee minimum execution time. In particular, 5% of the test cases (3 out of 56, without counting marginal differences) show that cf02 was not optimal in terms of runtime. The most significant of such test cases is the elastic model with $[q = 4, nf = 0]$. There are two reasons for this. Firstly, low level optimization can have a significant impact on actual performance. For example, the aggressive loop unrolling in *tens* eliminates operations on zeros and reduces the working set size by not storing entire temporaries; on the other hand, preserving the loop structure can maximize the chances of autovectorization. Secondly, memory constraints are critical, particularly the transformation strategy adopted when exceeding T_H . We will later thoroughly elaborate on all these aspects.



Fig. 7: Performance evaluation for the *mass* matrix. The bars represent speed-up over the original (unoptimized) code produced by the FEniCS Form Compiler.

Autovectorization. The discretizations employed result in inner loops and basis function tables of size multiple of the machine vector length. This, combined with the chosen compilation flags, promotes autovectorization in the majority of code variants. An exception is *quad* due to the presence of indirection arrays in the generated code. In *tens*, loop nests are fully unrolled, so the standard loop vectorization is not feasible; manual inspection of the compiled code suggests, however, that block vectorization ([Larsen and Amarasinghe 2000]) is often triggered. In *ufls*, *cf01*, and *cf02* the iteration spaces have similar structure (there are a few exceptions in *cf02* due to zero-elimination), with loop vectorization being regularly applied, as far as we could evince from compiler reports and manual inspection of assembly code.

Mass. We start with the simplest of the bilinear forms investigated, the mass matrix. Results are in Figure 7. We first notice that the lack of improvements when $q = 1$ is due to the fact that matrix insertion outweighs local assembly. As $q \geq 2$, *cf02* generally shows the highest speed-ups. It is worth noting how *auto* does not always select the fastest implementation: *auto* always opts for *tens*, while as $nf \geq 2$ *quad* would tend to be preferable. On the other hand, *cf02* always makes the optimal decision about whether applying pre-evaluation or not.



Fig. 8: Performance evaluation for the bilinear form of a *Helmholtz* equation. The bars represent speed-up over the original (unoptimized) code produced by the FEniCS Form Compiler.

Helmholtz. As happened with the mass matrix problem, when $q = 1$ matrix insertion still hides the cost of local assembly. For $q \geq 2$, the general trend is that cf02 outperforms the competitors. In particular, with

- $nf = 0$, the adoption of pre-evaluation by cf02 results in increasingly notable speed-ups over cf01, as q increases; tens is comparable to cf02, with auto making the right choice.
- $nf = 1$, auto picks tens; the choice is however sub-optimal when $q = 3$ and $q = 4$. This can indirectly be inferred from the large gap between cf01/cf02 and tens/auto: cf02 applies sharing elimination, but it avoids pre-evaluation.
- $nf = 2$ and $nf = 3$, auto reverts to quad, which would theoretically be the right choice (the flop count is much lower than in tens or what would be produced by pre-evaluation); however, the generated code suffers from the presence of indirection arrays, which break autovectorization and “traditional” code motion.

The sporadic slow-downs or only marginal improvements exhibited by ufls are imputable to the presence of sharing.

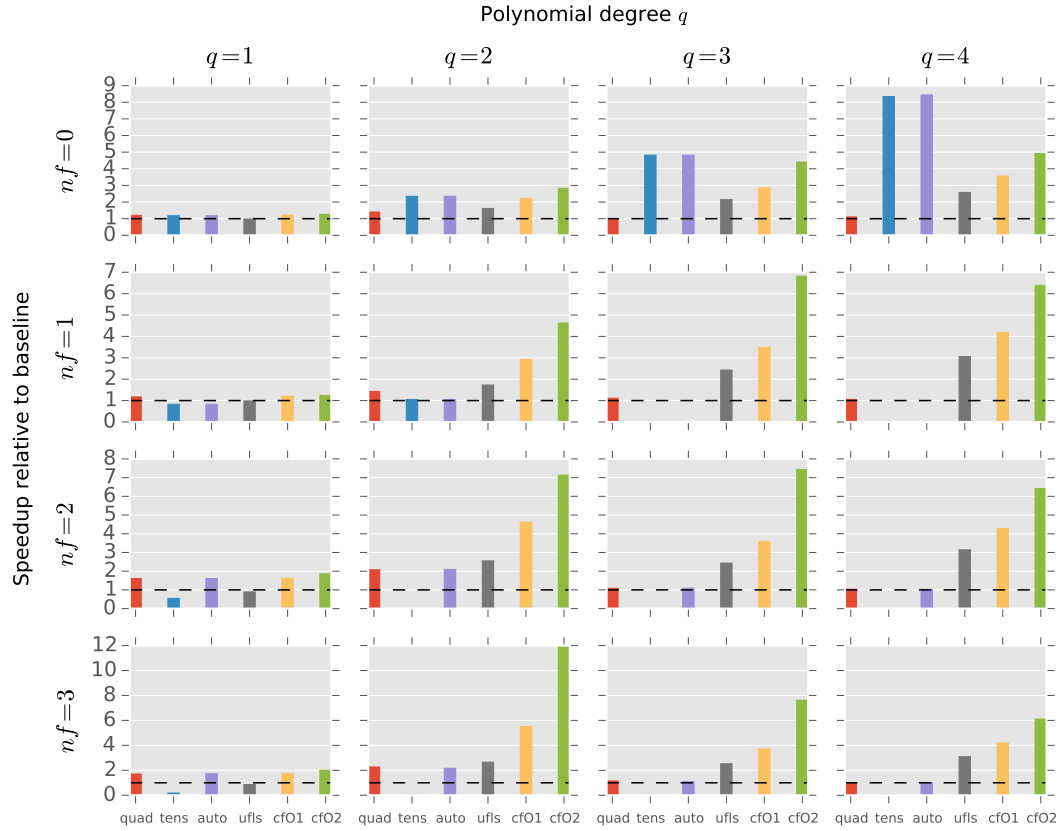


Fig. 9: Performance evaluation for the bilinear form arising in an *elastic* model. The bars represent speed-up over the original (unoptimized) code produced by the FEniCS Form Compiler.

An interesting experiment we performed was relaxing the memory threshold by setting it to $T_H = L3_{size}$. We found that this makes cf02 generally slower as $nf \geq 2$, with a maximum slow-down of $2.16\times$ with $\langle nf = 2, q = 2 \rangle$. The effects of not having a sensible threshold could even be worse in parallel runs, since the L3 cache is shared by the cores.

Elasticity. The results for the elastic model are displayed in Figure 9. The main observation is that cf02 never triggers pre-evaluation, although in some occasions it should. To clarify this, consider the test case $\langle nf = 0, q = 2 \rangle$, in which tens/auto show a considerable speed-up over cf02. cf02 finds pre-evaluation profitable – that is, actually capable of reducing the operation count – although it does not apply it because otherwise T_H would be exceeded. However, running the same experiments with $T_H = L3_{size}$ resulted in a dramatic improvement, even higher than that of tens. Our explanation is that despite exceeding T_H by roughly 40%, the save in operation count is so large ($5\times$ in this problem) that pre-evaluation would anyway be the optimal choice. This suggests that our model could be refined to handle the cases in which there is a significant gap between potential cache misses and save in flops.

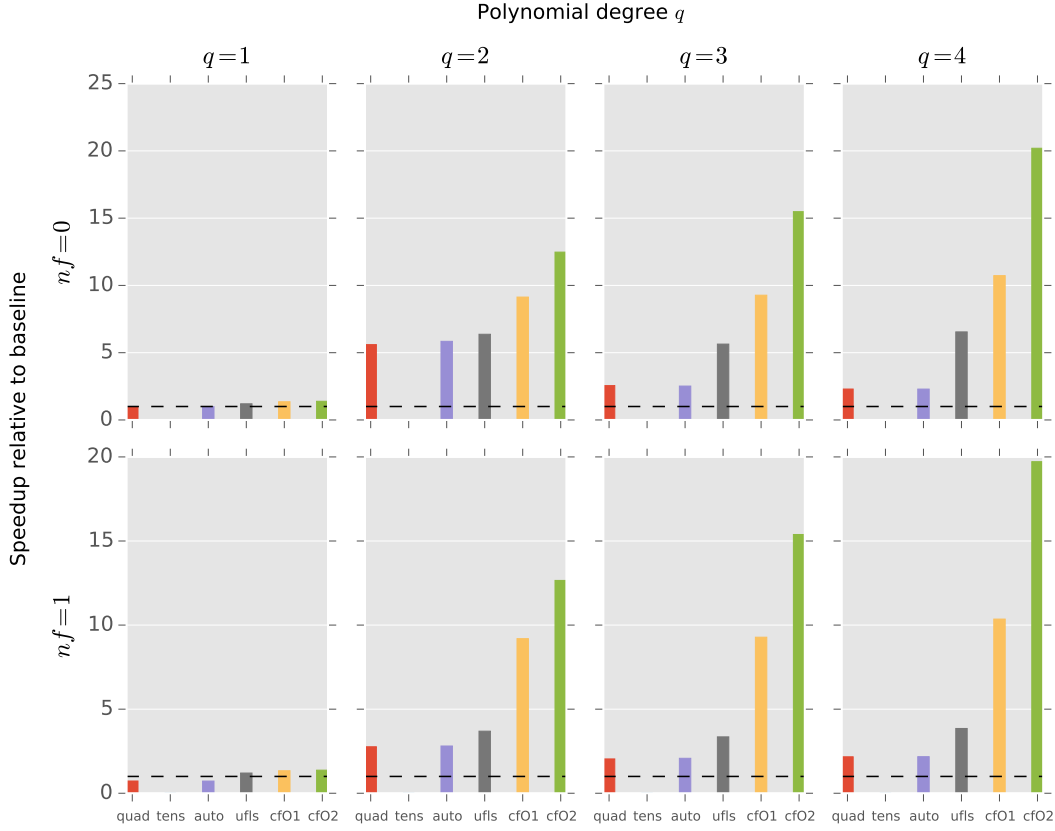


Fig. 10: Performance evaluation for the bilinear form arising in a *hyperelastic* model. The bars represent speed-up over the original (unoptimized) code produced by the FEn-iCS Form Compiler.

We also note that:

- the differences between cf02 and cf01 are due to systematic sharing elimination and the use of symbolic execution to avoid iteration over the zero-valued regions in the basis function tables
- when $n_f = 1$, auto prefers tens to quad, which leads to sub-optimal operation counts and execution times
- ufls generally shows better runtime behaviour than quad and tens. This is due to multiple facts, including avoidance of indirection arrays, preservation of loop structure, a more effective code motion.

Hyperelasticity. In the experiments on the hyperelastic model, shown in Figure 10, cf02 exhibits the largest gains out of all problem instances considered in this paper. This is a positive aspect: it means that our transformation algorithm scales with form complexity. The fact that all code transformation systems (apart from tens) show quite significant speed-ups suggests several points. Firstly, the baseline is highly inefficient: with forms as complex as in this hyperelastic model, a trivial translation of integration

routines into code should always be avoided since even one of the best general-purpose compilers available (Intel's on an Intel platform at maximum optimization level) is not capable of exploiting the structure inherent in the mathematical expressions generated. Secondly, the code motion strategy really makes a considerable impact. The sharing elimination performed by cf02 in each level of the loop nest ensures a critical reduction in operation count, which results in better execution times. In particular, at higher order, the main difference between ufls and cf02 is due to the application of this transformation to the outer product loop nest. Clearly, the operation count increases with q , and so do the speed-ups.

7. CONCLUSIONS

With this research we have set the foundation of optimal finite element integration. We have developed theory and implemented an automated system capable of applying it. The automated system, COFFEE, is integrated in Firedrake, a real-world framework for writing finite element methods. We believe the results are extremely positive. An open problem is understanding how to optimally handle non-linear loop nests. A second open problem is extending our methodology to classes of loops arising in spectral methods; here, the interaction with low level optimization will probably become stronger due to the typically larger working sets deriving from the use of high order function spaces. Lastly, we recall our work is publicly available and is already in use in the latest version of the Firedrake framework.

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