

# Optimizing Automated Finite Element Integration through Expression Rewriting and Code Specialization

Fabio Luporini, Imperial College London  
David A. Ham, Imperial College London  
Paul H.J. Kelly, Imperial College London

Abstract goes here

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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 incredibly popular over the last years. In these frameworks, the weak variational form of a given problem is expressed at high-level by means of a domain-specific language. Such a mathematical specification is suitably manipulated and then passed as input to a form compiler, whose goal is to generate a representation of local assembly operations. These operations numerically evaluate problem-specific integrals in order to compute so called local matrices and vectors, which represent the contributions from each element in the discretized domain to the equation solution. Local assembly code must be high performance: as the complexity of a variational form increases, in terms of number of derivatives, pre-multiplying functions, and polynomial order of the chosen function

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Author's addresses: Fabio Luporini & Paul H. J. Kelly, Department of Computing, Imperial College London; David A. Ham, Department of Computing and Department of Mathematics, Imperial College London;

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spaces, the resulting assembly kernels become more and more expensive, covering a significant fraction of overall computation run-time.

Achieving high performance implementations is, however, non-trivial. The complexity of mathematical expressions involved in the numerical integration, which varies from problem to problem, and the small size of the loop nest in which such integral is computed obstruct the optimization process. Also, traditional vendor compilers, such as *GNU's* and *Intel's*, fail at exploiting the structure inherent assembly expressions. This has led to development of a number of higher-level approaches to optimize local assembly kernels. In [Olgaard and Wells 2010], it is shown how automated code generation can be leveraged to introduce domain-specific optimizations, which a user cannot be expected to write “by hand”. [Kirby et al. 2005] and [Russell and Kelly 2013] have studied, instead, different optimization techniques based on a mathematical reformulation of the problem. In [Luporini et al. 2014], we have made one step forward by showing that different problems, on different platforms, require distinct set of transformations if close-to-peak performance needs to be obtained, and that low-level, domain-aware code transformations are essential to maximize instruction-level parallelism and register locality. The problem of optimizing local assembly routines has been tackled recently also for GPUs, for instance in [Knepley and Terrel 2013].

Our research has resulted in the development of a compiler, COFFEE<sup>1</sup>, fully integrated with the Firedrake framework. While clearly separating the mathematical domain, which remains captured in the higher-level form compiler, from the optimization process, COFFEE also aims to be platform-agnostic. The code transformations occur on an intermediate representation of the assembly code, which is ultimately translated into platform-specific code. Domain knowledge is exploited in two ways: for simplifying the implementation of a broad range of code transformations, and, obviously, to make them extremely effective. Domain knowledge is conveyed to COFFEE from the higher level (the form compiler in the case of Firedrake, although any user-provided code would be acceptable) through suitable annotations attached to the input. For example, when the input is in the form of an abstract syntax tree produced by the form compiler, specific nodes are decorated so as to drive the optimization process. Although COFFEE has been thought of as a multi-platform optimizing compiler, our performance evaluation so far has been restricted to standard CPU platforms only. We emphasize once more, however, that the transformations applicable by both the Expression Rewriter (Section 3) and the Code Specializer (Section 4) would work on generic accelerators as well.

In this paper, we build on the work presented in [Luporini et al. 2014] and present a novel structured approach to the optimization of automatically-generated finite element integration routines based on quadrature representation. We argue that peak performance can be achieved only by passing through a two-step optimization procedure: 1) expression rewriting, to minimize floating point operations, 2) and code specialization, to obtain, for instance, effective register utilization and SIMD vectorization. The code transformations introduced in [Luporini et al. 2014] are reused: as explained in Section 2.2, padding and data alignment, expression splitting, and vector-register tiling become sub-steps of code specialization; on the other hand, generalized loop-invariant code motion is a step of the expression rewriting process. More importantly, we complement and generalize our previous work with the following contributions.

Expression rewriting is based on a formal set of rewrite rules. Our first contribution consists of a framework that aggressively exploits associativity, distributivity, and commutativity of arithmetic operators to expose “hidden” loop-invariant sub-expressions.

<sup>1</sup>COFFEE stands for COmpiler For FinitE Element local assembly.

Secondly, we show how to make use of domain knowledge to avoid computation over zero-valued regions in vector-valued basis functions arrays, while preserving code vectorizability. These transformations will allow outperforming the results obtained in [Luporini et al. 2014] as well as those achievable by using FEniCS' built-in optimizations, presented in [Olgaard and Wells 2010].

At code specialization time, transformations are applied to maximize the exploitation of the underlying platform's resources, e.g. SIMD lanes. On top of the work in [Luporini et al. 2014], we provide a number of contributions. Firstly, we show the benefit of vector-expansion to achieve SIMD vectorization of otherwise scalar code. This is particularly useful in complex forms, like those based on hyperelasticity. Secondly, we answer an open problem in [Luporini et al. 2014] by providing an algorithm that automatically transforms an element matrix evaluation into a sequence of calls to BLAS' dense matrix multiplies. BLAS routines are known to perform far from peak performance when the involved arrays are small, which is almost always the case of low-order finite element methods. However, we will show that in corner, yet important cases, especially in forms characterized by pre-multiplying functions and relatively high-order function spaces, a BLAS-based execution strategy can be a successful. Finally, we introduce a model-driven, dynamic autotuner that automatically and transparently compose the set of code transformations that are likely to maximize the performance of a given problem. The main challenge with the autotuner is to maintain, for any possible problem, the search space reasonably small, although comprising the most effective code variants, so that the overhead, which impacts the run-time, is negligible.

Expression rewriting and code specialization have been implemented in COFFEE and are fully operating. Therefore, to testify the goodness of our approach, we provide an extensive and unprecedented performance evaluation in a number of forms of increasing complexity, including problems based on hyperelasticity operators. We characterize our problems by varying polynomial order of the employed function spaces and number of pre-multiplying functions. To clearly distinguish the improvement achieved by this work, we will compare four sets of code variants, for each problem instance: 1) unoptimized code, i.e. a local assembly routine as returned from the form compiler; 2) code optimized by FEniCS, i.e. the work in [Olgaard and Wells 2010]; 3) code optimized as described in [Luporini et al. 2014]; code optimized by expression rewriting and code specialization as described in this paper. Notable performance improvements of 4) over 1), 2) and 3) are reported and detailed.

## 2. PRELIMINARIES

### 2.1. Quadrature for Finite Element Local Assembly

We summarize the basic concepts sustaining the finite element method following the notation adopted in [Olgaard and Wells 2010] and [Russell and Kelly 2013]. We consider the weak formulation of a linear variational problem

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

where  $a$  and  $L$  are called bilinear and linear form, respectively. The set of *trial* functions  $U$  and the set of *test* functions  $V$  are discrete function spaces. For simplicity, we assume  $U = V$  and  $\{\phi_i\}$  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  $u$

$$A\mathbf{u} = b \tag{2}$$

in which  $A$  and  $b$  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  $b$  are computed in the so called assembly phase. Then, in a subsequent phase, the linear system is solved, usually by means of an iterative method, and  $\mathbf{u}$  is eventually evaluated.

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 the paper: this is about computing the contributions that an element in the discretized domain provide to the approximated solution of the equation. Global assembly, on the other hand, is the process of suitably “inserting” such contributions in  $A$  and  $b$ .

Without loss of generality, we illustrate local assembly in a real example, the evaluation of the local assembly (or, equivalently, 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  $\Omega$  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  $L$  can be determined in an analogous way.

Quadrature schemes are conveniently 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 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 representation 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  $\Omega$ ,  $n$  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.

In the next sections, we will often refer to the (local) element matrix evaluation, such as Equation 7 for the weighted Laplace operator, as the *assembly expression* of the variational problem.

## 2.2. COFFEE: a Compiler for Optimizing Quadrature-based Finite Element Integration

If high performance code needs to be generated, assembly expressions must be optimized with regards to three interrelated aspects: 1) arithmetic intensity, 2) instruction-

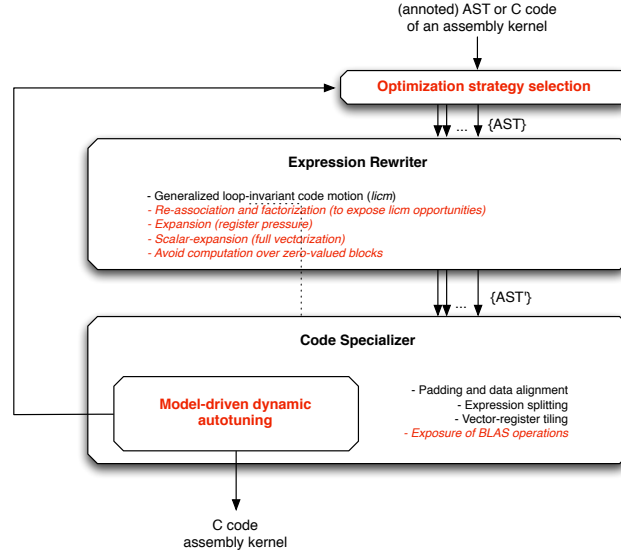


Fig. 1: Outline of COFFEE

level parallelism, and 3) data locality. In this paper, we tackle these three points building on our previous work ([Luporini et al. 2014]).

COFFEE is a mature, platform-independent compiler capable of optimizing local assembly code. Its high-level structure can be outlined as in Figure 1. The input is either suitably-annotated C code, explicitly provided by the user, or a decorated abstract syntax tree (henceforth AST) representation of an assembly kernel, automatically generated by the higher level in the stack. We have integrated COFFEE with the Firedrake framework; here, the input to COFFEE is originated by the FEniCS Form Compiler in the form of an AST. Decoration of special AST nodes, or equivalently annotation of C code, is extensively used to convey domain knowledge to COFFEE. This is used to introduce more effective, specialized optimizations, as well as to simplify implementation.

Two conceptually distinct software modules can be individuated: the Expression Rewriter and the Code Specializer. The former targets arithmetic intensity. Its role is to transform the assembly expression and, therefore, the enclosing loop nest, so as to minimize the number of floating point operations that are performed to evaluate the element matrix (or vector). The latter is tailored to optimizing for instruction-level parallelism, particularly SIMD vectorization, and data (register) locality. The Expression Rewriter manipulates and transforms the original AST, which is then provided to the Code Specializer. As described later, we have invested some effort to ensure that the code transformations applied in the expression rewriting stage do not break any code specialization opportunity. This for example would not be the case if the Expression Rewriter coincided with the FEniCS Form Compiler’s built-in optimization system; we will clarify this aspect in Section 3.3.

To neatly distinguish the contributions of this paper from those in [Luporini et al. 2014], in this section we summarize the results of our previous work. Moreover, in Section 5, we will explicitly compare the performance achieved with the transformations presented in this paper to [Luporini et al. 2014] (as well as to FEniCS’ built-in optimizations).

In our previous work, we have demonstrated the effectiveness of a set of optimizations for finite element quadrature-based integration routines originated through automated code generation. We have also shown how different subset of optimizations are needed to achieve close-to-peak performance in different problems. In particular, we can summarize our study as follows

- *Generalized Loop-invariant Code Motion*. Compiler’s loop-invariant code motion algorithms may not be general enough to optimize assembly expressions, in which different sub-expressions are invariant with respect to more than one loop in the enclosing nest. As briefly described in Section 3, we work around this limitation, while also achieving vectorization of invariant code.
- *Padding and data alignment*. The small size of the loop nest require all of the involved arrays to be padded to a multiple of the vector register length so as to maximize the effectiveness of SIMD code. Data alignment can be enforced as a consequence of padding.
- *Vector-register Tiling*. Blocking at the level of vector registers, which we perform exploiting the specific memory access pattern of the assembly expressions (i.e. a domain-aware transformation), improves data locality beyond traditional unroll-and-jam optimizations. This is especially true for relatively high polynomial order (i.e. greater than 2) or when pre-multiplying functions are present.
- *Expression Splitting*. In certain assembly expressions the register pressure is significantly high: when the number of basis functions arrays (or, equivalently, temporaries introduced by loop-invariant code motion) and constants is large, spilling to L1 cache is a consequence for architectures with a relatively low number of logical registers (e.g. 16/32). We exploit sum’s associativity to “split” the assembly expression into multiple sub-expressions, which are computed individually.

In Figure 1, we show where these transformations are logically applied in COFFEE; also, the contributions of this work are highlighted. In the next two sections, we describe the new functionalities of, respectively, the Expression Rewriter and the Code Specializer.

### 3. EXPRESSION REWRITING

As summarized in 2.2, loop-invariant code motion is the key to reduce the computational intensity of an assembly expression. The Expression Rewriter (henceforth ER) that we have designed and implemented in COFFEE enhances this technique by making two steps forward, which allow more redundant computation to be avoided.

Firstly, exploiting arithmetic operations properties like associativity, distributivity, and commutativity, it manipulates the original expression to expose more opportunities to the code hoister. There are many possibilities of rewriting an expression, and the search space can quickly become too big. Therefore, one problem we solve is finding a sufficiently simple yet systematic way of maximizing the amount of loop-invariant operations in an expression. In Section 3.1, we formalize the set of rewrite rules that COFFEE follows to transform an expression.

Secondly, the ER re-structures the loop nest so as to eliminate arithmetic operations over array columns that are statically known to be zero-valued. Zero columns in tabulated basis functions appear, for example, when taking derivatives on a reference element or when using mixed elements. A code transformation eliminating floating point operations on zeros was presented in [Olgaard and Wells 2010]; however, the issue with it is that by using indirection arrays in the generated code, it breaks many of the optimizations that can be applied at the Code Specializer level, including SIMD vectorization. In Section 3.3, we show a novel approach to avoiding computation on zeros based on symbolic execution.

```

for (int i=0; i<I; ++i) {
  // Coefficient evaluation at point i
  for (int r=0; r<T; ++r) {
    f0 += ...; f1 += ...; ...;
  }
  // Test functions
  for (int j=0; j<T; ++j)
    // Trial functions
    for (int k=0; k<T; ++k)
      M[j][k] += (((a*f0*A[i][j]+b*f1*B[i][j])*A[i][k]*g)+
                  ((A[i][k]/c)*A[i][j])+
                  (((d*D[i][k]+e*E[i][k])*A[i][j])*f)
                  )*det*W[i];
}

```

(a) Original code

```

for (int i=0; i<I; ++i) {
  for (int r=0; r<T; ++r) {
    f0 += ...; f1 += ...; ...;
  }
  double T1[T], T2[T];
  for (int r=0; r<T; ++r) {
    T1[r] = ((f0*a*A[i][r])+(f1*b*B[i][r]));
    T2[r] = ((d*D[i][r])+(e*E[i][r]));
  }
  for (int j=0; j<T; ++j)
    for (int k=0; k<T; ++k)
      M[j][k] += ((T1[j]*A[i][k]*g)+
                  ((A[i][k]/c)*A[i][j])+
                  (T2[k]*A[i][j]*f))*det*W[i];
}

```

(b) Invariant code

```

for (int i=0; i<I; ++i) {
  for (int r=0; r<T; ++r) {
    f0[i] += ...; f1[i] += ...; ...;
  }
  k0[i] = f0[i]*a; k1[i] = f1[i]*b;
}
for (int i=0; i<I; ++i) {
  double T1[T], T2[T];
  for (int r=0; r<T; ++r) {
    T1[r] = ((k0[i]*A[i][r])+(k1[i]*B[i][r]));
    T2[r] = ((d*D[i][r])+(e*E[i][r]));
    T3[r] = ((A[i][r]/c)+T2[r]*f);
  }
  for (int j=0; j<T; ++j)
    for (int k=0; k<T; ++k)
      M[j][k] += ((T1[j]*A[i][k]*g)+
                  (T3[k]*A[i][j]))*det*W[i];
}

```

(c) Factorized code

```

for (int i=0; i<I; ++i) {
  for (int r=0; r<T; ++r) {
    f0[i] += ...; f1[i] += ...; ...;
  }
  k0[i] = f0[i]*a; k1[i] = f1[i]*b;
}
for (int i=0; i<I; ++i) {
  double T1[T], T2[T];
  for (int r=0; r<T; ++r) {
    T1[r] = ((k0[i]*A[i][r])+(k1[i]*B[i][r]));
    T2[r] = ((d*D[i][r])+(e*E[i][r]));
    T3[r] = ((A[i][r]/c)+T2[r]*f);
  }
  for (int j=0; j<T; ++j)
    for (int k=0; k<T; ++k)
      M[j][k] += ((T1[j]*A[i][k]*g)+
                  (T3[k]*A[i][j]))*det*W[i];
}

```

(d) Scalar-expanded code

Fig. 2: Original, invariant, factorized, and then scalar-expanded code.

### 3.1. Objectives of the Expression Rewriter

Consider the element matrix computation in Figure 2(a), which is an excerpt from a Burgers problem. The assembly expression, produced by the FEniCS Form Compiler, has been deliberately simplified, and code details have been omitted for brevity and readability. In practice, assembly expressions can be much more complex, for example depending on the differential operators employed in the variational form; however, this example is representative enough for highlighting patterns that are common in a large class of problems.

A first glimpse of the code suggests that the sub-expression  $a*f0*A[i][j]+b*f1*B[i][j]$  is invariant with respect to the innermost (trial functions) loop  $k$ , so it can be hoisted at the level of the outer loop  $j$  to avoid redundant computation. This is indeed a standard compiler transformation, supported by any available compilers, so, in principle, there should be no need to transform the source code explicitly. With a closer look we notice that the sub-expression  $d*D[i][k]+e*E[i][k]$  is also invariant, although, this time, with respect to the outer (test functions) loop  $j$ . In [Luporini et al. 2014], we have showed that available compilers limit the search for code motion opportunities to the innermost loop of a given loop nest. Moreover, the lack of cost models to ascertain both the optimal place where to hoist an expression and whether or not vectorizing it at the price of extra temporary memory is a fundamental limiting factor. The *generalized loop-invariant code motion* technique that we implemented in COFFEE, leading to the code in Figure 2(b), addressed these limitations, which are critical in the case of non-trivial assembly expressions, resulting in run-time improvements up to  $3\times$ .

In this paper, we target particularly complex variational forms for which a more aggressive transformation is required. We generalize the problem of finding and hoisting

invariant sub-expressions by formulating the following critical question: *how an assembly expression should be rewritten so as to minimize both floating point operations and data movement?* To minimize floating point operations, in terms of instructions executed, it is important to reduce the absolute number of arithmetic operations to evaluate the element matrix as well as to achieve full vectorization of the assembly loop nest.

We start considering the case of assembly expressions that, after generalized loop-invariant code motion has been applied, still “hide” opportunities for code hoisting. By examining again the code in Figure 2(b), we notice that the basis function array  $A$  iterating along the  $[i, j]$  loops appears twice in the expression. By expanding the products in which  $A$  is accessed and applying sum commutativity, we can factorize the expression. This has two effects: firstly, it reduces the number of arithmetic operations performed; secondly, and most importantly, it exposes a new sub-expression  $A[i][k]/c+T2[k]*f$  invariant with respect to loop  $j$ . Consequently, hoisting can be performed, resulting in the code in Figure 2(c). In general, exposing factorization opportunities requires traversing the whole expression tree, and then expanding and moving terms. It also needs heuristics to select a factorization strategy: there may be different opportunities of reorganizing sub-expressions, and, in our case, the best is the one that maximizes the invariant code eventually disclosed. We will discuss this aspect formally in Section 4.

As a second observation, we note that integration-dependent expressions are inherently executed as scalar code. For example, the  $f0*a$  and  $f1*b$  products in Figure 2(c) depend on the loop along quadrature points; these operations are performed in a non-vectorized way at every  $i$  iteration. This is not an issue in our running example, where scalar computation represents a small percentage of the total, but it becomes a concrete problem in complicated forms, like those at the heart of hyperelasticity (which we evaluate in Section 5). In such forms, the amount of computation independent of both test and trial functions loops is so large that it has a significant impact on the runtime, despite being executed only  $O(I)$  times (with  $I$  number of quadrature points). We have therefore implemented an algorithm to scalar-expand integration-dependent expressions, which leads to codes as in Figure 2(d).

The third point concerns the register pressure induced by the assembly expression. Once the code has been optimized for arithmetic intensity, it is important to think about how the transformations impacted register allocation. Assume the local assembly kernel is executed on a state-of-the-art CPU architecture having 16 logical registers, e.g. an Intel Haswell. Each value appearing in the expression is loaded and kept in a register as long as possible. In Figure 2(d), for instance, the scalar value  $g$  is loaded once, whereas the term  $\det*W[i]$  is precomputed and loaded in a register at every  $i$  iteration. This implies that at every iteration of the  $jk$  loop nest, 12% of the available registers are spent just to store values independent of test and trial functions loops. In more complicated expressions, the percentage of registers destined to store such constant terms can be even higher. Registers are, however, a precious resource, especially when evaluating compute-intensive expressions. The smaller is the number of available free registers, the worse is the instruction-level parallelism achieved: for example, a shortage of registers can increase the pressure on the L1 cache (i.e. it can worsen data locality), or it may prevent the effective application of standard transformations, e.g. loop unrolling. We aim at relieving this problem by suitably expanding terms and introducing, where necessary, additional temporary values. We illustrate this in the following example.

Consider a variant of the Burgers local assembly kernel, shown in Figure 3(a). This is still a representative, simplified example. We can easily distribute  $\det*W[i]$  over the three operands on the left-hand side of the multiplication, and then absorb it in



```

for (int i=0; i<I; ++i) {
  double T1[T];
  for (int r=0; r<T; ++r) {
    T1[r] = ((a*A[i][r])+(b*B[i][r]));
  }
  for (int j=0; j<T; ++j)
    for (int k=0; k<T; ++k)
      M[j][k] += (((T1[j]*A[i][k])+(T1[k]*A[i][j]))*g+(T1[j]*A[i][k]))*det*W[i];
}

```

(a) Expandable code

```

for (int i=0; i<I; ++i) {
  double T1[T];
  for (int r=0; r<T; ++r) {
    T1[r] = ((a*A[i][r])+(b*B[i][r]))*det*W[i];
  }
  for (int j=0; j<T; ++j)
    for (int k=0; k<T; ++k)
      M[j][k] += (T1[j]*A[i][k]+T1[k]*A[i][j])*g+(T1[j]*A[i][k]);
}

```

(b) Expanded 1 code

```

for (int i=0; i<I; ++i) {
  double T1[T], T2[T];
  for (int r=0; r<T; ++r) {
    T1[r] = ((a*A[i][r])+(b*B[i][r]))*det*W[i];
    T2[r] = T1[r]*g;
  }
  for (int j=0; j<T; ++j)
    for (int k=0; k<T; ++k)
      M[j][k] += (T2[j]*A[i][k])+(T2[k]*A[i][j])+(T1[j]*A[i][k]);
}

```

(c) Expanded 2 code

Fig. 3: Expanding code.

the pre-computation of the invariant sub-expression stored in T1, resulting in code as in Figure 3(b). Freeing the register destined to the constant  $g$  is less straightforward: we cannot absorb it in T1 as we did with  $\text{det} * W[i]$  since the same array is accessed in  $(T1[j] * A[i][k])$ . The solution is to add another temporary as in Figure 3(c). Generalizing, this is a problem of data dependencies: to solve it, we use a dependency graph in which we add a direct edge from identifier A to identifier B to denote that the evaluation of B depends on A. The dependency graph is initially empty, and it is updated every time a new temporary is created by either loop-invariant code motion or expansion of terms. The dependency graph is then queried to understand when expansion can be performed without resorting to new temporary values. This aspect is formalized in the next section.

### 3.2. Rewrite Rules

In general, assembly expressions produced by automated code generation can be much more complex than those we have used as examples, with dozens of terms involved (basis function arrays, derivatives, coefficients, ...) and hundreds of (nested) arithmetic operations. Our goal is to establish a portable, unified, platform-independent, and systematic way of reducing the computational strength of an expression exploiting the intuitions described in the previous section. This *expression rewriting* should be simple; definitely, it must be robust to be integrated in an optimizing domain-specific compiler capable of supporting real problems. In other words, we look for an algorithm capable of transforming a plain assembly expression by applying 1) generalized loop-invariant code motion, 2) non-trivial factorization and re-association of sub-expressions, and 3) expansion of terms; after that, it should perform scalar-expansion to achieve full vectorization of the assembly code.

We centre such an algorithm around a set of rewrite rules. These rules drive the transformation of an expression, prescribe where invariant sub-expressions will be moved (i.e. at what level in the loop nest), and track the propagation of data dependencies. When applying a rule, the state of the loop nest must be updated to reflect, for example, the use of a new temporary and new data dependencies. We define the state of a loop nest as  $L = (\sigma, G)$ , where  $G = (V, E)$  represents the dependency graph, while  $\sigma : Inv \rightarrow S$  maps invariant sub-expressions to identifiers of temporary arrays. The notation  $\sigma_i$  refers to invariants hoisted at the level of loop  $i$ . We also introduce the

Rule	Precondition
$[a_i \cdot b_j]_{(\sigma, G)} \rightarrow [a_i \cdot b_j]_{(\sigma, G)}$	
$[(a_i + b_j) \cdot \alpha]_{(\sigma, G)} \rightarrow [(a_i \cdot \alpha + b_j \cdot \alpha)]_{(\sigma, G)}$	
$[a_i \cdot b_j + a_i \cdot c_j]_{(\sigma, G)} \rightarrow [(a_i \cdot (b_j + c_j))]_{(\sigma, G)}$	
$[a_i + b_i]_{(\sigma, G)} \rightarrow [t_i]_{(\sigma', G')}$	$t_i = \sigma_{i_0}[\iota'_i/a_i + b_i], G' = (V \cup t_i, E \cup \{(t_i, a_i), (t_i, b_i)\})$
$[(a_i \cdot b_j) \cdot \alpha]_{(\sigma, G)} \rightarrow [t_i \cdot b_j]_{(\sigma', G')}$	$\#(b_j) > \#(a_i), t_i = \sigma_{i_0}[\sigma[\perp/a_i]/a_i \cdot \alpha], a_i \notin in(G),$ $G' = (V \cup t_i, E \cup \{(t_i, a_i), (t_i, \alpha)\})$
$[(a_i \cdot b_j) \cdot \alpha]_{(\sigma, G)} \rightarrow [t_i \cdot b_j]_{(\sigma', G')}$	$\#(b_j) > \#(a_i), t_i = \sigma_{i_0}[\iota'_i/a_i \cdot \alpha], a_i \in in(G),$ $G' = (V \cup t_i, E \cup \{(t_i, a_i), (t_i, \alpha)\})$

Fig. 4: Rewrite rules.

*conditional hoister operator*  $\square$  on  $\sigma$  such that

$$\sigma[v/x] = \begin{cases} \sigma(x) & \text{if } x \in Inv; v \text{ is ignored} \\ v & \text{if } x \notin Inv; \sigma(x) = v \end{cases}$$

That is, if the invariant expression  $x$  has already been hoisted,  $\square$  returns the temporary identifier hosting its value; otherwise,  $x$  is hoisted and a new temporary  $v$  is created. There is a special case when  $v = \perp$ , used for *conditional deletion* of entries in  $\sigma$ . Specifically

$$\sigma[\perp/x] = \begin{cases} \sigma(x) & \text{if } x \in Inv; \sigma = \sigma \setminus (x, \sigma(x)) \\ v & \text{if } x \notin Inv; v \notin S \end{cases}$$

In other words, the invariant sub-expression  $x$  is removed and the temporary identifier that was hosting its value is returned if  $x$  had been previously hoisted; otherwise, a fresh identifier  $v$  is returned. This is useful to express updates of hoisted invariant sub-expressions when expanding terms.

In the following, a generic (sub-)expression is represented with roman letter  $a, b, \dots$ ; constant terms are considered a special case, so greek letters  $\alpha, \beta$  are used instead. The iteration vector  $i = [i_0, i_1, \dots]$  is the ordered sequence of the indices of the loops enclosing an (sub-)expression. We will refer to  $i_0$  as the outermost enclosing loop. The notation  $a_{i_0}$ , therefore, indicates that the expression  $a$  assume distinct values while iterating along the loops in  $i$ ; its outermost loop is silently assumed to be  $i_0$ .

Rewrite rules for expression rewriting are provided in Figure 4; obvious rules are omitted for brevity. The Expression Rewriter applies the rules while performing a depth-first traversal of the assembly expression tree. Given an arithmetic operation between two sub-expressions (i.e. a node in the expression tree), we first need to find an applicable rule. There cannot be ambiguities: only one rule can be matched. If the preconditions of the rule are satisfied, the corresponding transformation is performed; otherwise, no rewriting is performed, and the traversal proceeds. As examples, it is possible to instantiate the rules in the codes shown in Figures 2(a) and 3(a); eventually, the optimized codes in Figures 2(c) and 3(c) are obtained, respectively.

```

void burgers(double M[6][6],
             double **coordinates,
             double **coeff0) {
    // Calculate determinant of jacobian
    // (det) using the coordinates field

    // Define tabulation of basis functions
    // (and their derivatives) arrays
    ...
    @coffee mfs[3, 5]
    static const double D[6][6] =
        {{0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0}};

    for (int i=0; i<6; ++i) {
        ...
        double T1[6], T2[6];
        for (int r=0; r<6; ++r) {
            T1[r] = a*A[i][r]+b*B[i][r];
            T2[r] = d*D[i][k]+e*E[i][k];
        }
        for (int j=0; j<6; ++j)
            for (int k=0; k<6; ++k)
                M[j][k] += (T1[j], T2[k], A[i][j], ...)
    }
}

```

(a) Factorized, showing zeros, code

```

void burgers(double M[6][6],
             double **coordinates,
             double **coeff0) {
    // Calculate determinant of jacobian (det)
    // using the coordinates field

    // Define tabulation of basis functions
    // (and their derivatives) arrays
    ...
    @coffee mfs[3, 5]
    static const double D[6][6] =
        {{0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0},
         {0.0, 0.0, 0.0, -1.0, 0.0, 1.0}};

    for (int i=0; i<6; ++i) {
        ...
        double T1[6], T2[6];
        for (int r=0; r<6; ++r) {
            T1[r] = a*A[i][r]+b*B[i][r];
            T2[r] = d*D[i][k]+e*E[i][k];
        }
        for (int j0=0; j0<3; ++j0)
            for (int k0=0; k0<3; ++k0)
                M[j0+3][k0+3] += f(T1[j0+3], A[i][k0+3], ...);
        for (int j1=0; j1<3; ++j1)
            for (int k1=0; k1<6; ++k1)
                M[j1][k1] += g(T2[k1], A[i][j1+3], ...);
    }
}

```

(b) Factorized, skipping zeros, code

Fig. 5: Without and with skipping zeros

To what extent should rewrite rules be applied is a question that cannot be answered in general. In some problems, a full rewrite of the expression may be the best option; in other cases, on the other hand, an aggressive expansion of terms, for example, may lead to high register pressure in the loops computing invariant terms, worsening the performance. In Section 4.3 we explain how to leverage the Code Specializer to select a suitable rewriting strategy for the problem at hand.

### 3.3. Avoiding Iteration on Zero-blocks by Symbolic Execution

We aim at skipping arithmetic operations over blocks of zero-valued entries in basis functions (and their derivatives) arrays. Zero-valued columns arise, for example, when taking derivatives on a reference element and when employing mixed elements. In [Olgaard and Wells 2010], a technique to avoid operations on zero-valued columns based on the use of indirection arrays was described (e.g.  $A[B[i]]$ , where  $A$  is a tabulated basis function and  $B$  a map from loop iterations to non-zero columns in  $A$ ) and implemented in the context of FEniCS. We will evaluate our approach and compare it to this pioneering work in Section 5. Essentially, our strategy avoids indirection arrays in the generated code, which otherwise would break the optimizations applicable at the Code Specializer level, including SIMD vectorization.

Consider Figure 5(a), which is an enriched version of the Burgers excerpt in Figure 2(b). The code is instantiated for the specific case of polynomial order 1, Lagrange elements on a 2D mesh. The array  $D$  represents a tabulated derivative of a basis function at the various quadrature points. There are four zero-valued columns. Any multiplications or additions along these columns could (should) be skipped to avoid irrelevant floating point operations. The solution adopted in [Olgaard and Wells 2010] is not to generate the zero-valued columns (i.e. to generate a dense  $6 \times 2$  array), to reduce the size of the iteration space over test and trial functions (from 6 to 2), and to use an indirection array (e.g.  $ind = \{3, 5\}$ ) to update the right entries in the element tensor  $A$ . This prevents, among the various optimizations, effective SIMD vectorization, because memory loads and store would eventually reference non-contiguous locations.

Our approach is based on using domain knowledge and symbolic execution. We discern the origin of zero-valued columns: for example, those due to taking derivatives on the reference element from those inherent to using mixed (vector) elements. In the running Burgers example, the use of vector function spaces require the generation of a zero-block (columns 0, 1, 2 in the array D) to correctly evaluate the local element matrix while iterating along the space of test and trial functions. The two key observations are that 1) the number of zero-valued columns caused by using vector function spaces is, often, much larger than that due to derivatives, and 2) such columns are contiguous in memory. Based on this, we aim at avoiding iteration only along the block of zero-valued columns induced by mixed (vector) elements.

We achieve our goal by symbolic execution. The Expression Rewriter expects some indication in the input exposing the location of the zero-valued columns due to mixed (vector) function spaces, in each tabulated basis function. This indication comes either in the form of code annotation, if the input to COFFEE were provided as pure C (as shown in Figure 5(a)), or by suitably decorating basis functions nodes, if the input were an abstract syntax tree. Then, the rewrite rules are applied and each statement is executed symbolically. For example, consider the assignment  $T2[r] = d*D[i][k] + e*E[i][k]$  in Figure 5(a). Array D has non-zero-valued columns in positions  $NZ_D = [3, 5]$ ; we also assume array E has non-zero-valued columns in positions  $NZ_E = [0, 2]$ . Multiplications by scalar values do not affect the propagation of non-zero-valued columns. On the other hand, when symbolically executing the sum of the two operands  $d*D[i][k]$  and  $e*E[i][k]$ , we track that the target identifier T2 will have non-zero-valued columns in positions  $NZ_D \cup NZ_E = [0, 5]$ . Eventually, exploiting the  $NZ$  information computed and associated with each identifier, we split the original assembly expression into multiple sets of sub-expressions, each set characterized by the same range of non-zero-valued columns. In our example, assuming that  $NZ_{T1} = [3, 5]$  and  $NZ_A = [3, 5]$ , there are two of such sets, this leads to the generation of two distinct iteration spaces, one for each set, as in Figure 5(b).

#### 4. CODE SPECIALIZATION

Code specialization provides a range of code transformations tailored to optimizing for instruction-level parallelism and register locality. As summarized in Section 2.2 and described in [Luporini et al. 2014], padding and data alignment, expression splitting, and outer-product vectorization, which is a domain-aware implementation of vector-register tiling, are examples of optimizations that the Code Specializer is capable of applying. In this paper, we enrich this set of transformations as explained in the following sections.

##### 4.1. Padding and Data Alignment Revisited

Padding and data alignment as described in [Luporini et al. 2014] must be refined for the case in which computation over zero-valued columns is avoided. We recall effective SIMD vectorization can be achieved only if the innermost loop size is a multiple of the vector register length. In the case of an AVX instruction set, for example, we want the size of innermost loops to be multiples of 4 (vector registers can fit up to four double-precision floats). Moreover, efficient loads and stores can be issued only if all of the involved arrays' base addresses are multiple of the vector register length.

Consider again the code in Figure 5(b). The arrays in the loop nest  $[j1, k1]$  can be padded and the right bound of loop k1 can be safely increased to 8: eventually, values computed in the region  $M[0 : 3][6 : 8]$  will be discarded. Then, by explicitly aligning arrays and using suitable pragmas (e.g. `#pragma simd` for the Intel compiler), effective SIMD auto-vectorization can be obtained.

There are some complications in the case of loops  $[j0, k0]$ . Here, increasing the loop bound to 4, despite being still safe, has no effect: for instance, the starting addresses of load instructions are  $T1[3]$  and  $A[i][3]$ , which are not aligned. One solution is to start iterating from the closest index that would ensure data alignment: in this specific case,  $k0 = 0$ , which would mean losing the effect of expression rewriting. Another possibility is to attain to non-aligned accesses. COFFEE can generate code for both situations, so we leave the autotuner, described in Section 4.3, in charge of determining the optimal transformation.

Note that in some cases it is not even safe to increase loop bounds, since extra iterations would access non-zero entries in the local element matrix  $M$ . In such a situation, there may be no possibility of restoring data alignment at all.

#### 4.2. Exposing Linear Algebra Operations

In [Luporini et al. 2014], we introduced the idea of transforming the element matrix evaluation into a sequence of calls to highly-optimized dense matrix-matrix multiply routines (henceforth DGEMM), for instance MKL or ATLAS BLAS. We compared COFFEE's optimizations with hand-written MKL-based kernels, showing how the small sizes of the involved arrays impair DGEMM routines, which are usually tuned for large arrays. The study was conducted only in the case of a specific Helmholtz problem. There are scenarios, however, in which tabulated basis functions sizes grow up to a point for which turning to BLAS may actually lead to better performance. For example, this can happen when relatively-high polynomial orders are used or if coefficients are present in the form, since they are both responsible for the size of tabulated basis functions. To explore these scenarios, we have developed an algorithm that reduces any assembly expression evaluation to a sequence of DGEMM calls.

Here, we informally provide the main steps of the algorithm. By fully applying the rewrite rules in Figure 4, an assembly expression is reduced to a summation, over each quadrature point, of outer products along the test and trial functions. Each outer product is then isolated, i.e. the assembly expression is split into chunks, each chunk representing an outer product over test and trial functions. Statements in the bodies of the surrounding loops (e.g. coefficients evaluation at a quadrature point, temporaries introduced by expression rewriting) are vector-expanded and hoisted completely outside of the loop nest, similarly to what we have described in Section 3.1. This renders perfect the loop nest; that is, there is no intervening code among the various loops. The element matrix evaluation has now become a sequence of dense matrix-matrix multiplies (transposition aside)

$$A_{jk} = \sum_i x_{0_{ij}} \cdot y_{0_{ik}} + \sum_i x_{1_{ij}} \cdot y_{1_{ik}} + \dots$$

where  $x_0, x_1, y_0, y_1, \dots$  are tabulated basis functions or vector-expanded temporaries introduced at expression rewriting time. Eventually, the storage layout of the involved operands is changed so as to be conforming to the BLAS interface (e.g. two dimensional arrays are flatten as one dimensional arrays). The translation of each loop nest into a DGEMM call is the last, straightforward step.

#### 4.3. Model-driven Dynamic Autotuning

We have demonstrated in [Luporini et al. 2014] that an optimal set of code transformations does not exist. What sequence of transformations applying to a problem to optimize its performance depends on a broad range of factors, including mathematical structure of the input form, polynomial order of employed function spaces, presence of

pre-multiplying functions, and, of course, the characteristics of the underlying architecture.

In [Luporini et al. 2014], we proposed a simple cost model that COFFEE could use to choose, given a problem, the transformations that were likely to maximize the performance. By having added a significant number of options to the set of possible optimizations, the selection problem is now far more challenging. The sole Expression Rewriter, for instance, could apply rewrite rules up to a set of pre-established depths, leading to the generation of many possible code variants.

We tackle this problem by compiler autotuning. For each problem, not only does it allow to determine the best combination of transformations out of the set presented so far, also it enables exploring parametric low-level optimizations, such as loop unroll, unroll-and-jam, and interchange, by trying multiple unroll factors and loop permutations. By leveraging the cost model defined in our previous study, domain-awareness, and a set of heuristics, we manage to keep the autotuner overhead at a minimum, whilst achieving significant speed ups over the purely cost-model-based implementation. In particular, our autotuner usually requires order of seconds to determine the fastest kernel implementation, a negligible overhead when it comes to iterate over real-life unstructured meshes, which can contain up to trillions of elements (e.g. [Rossinelli et al. 2013]).

The structure of the autotuner is outlined in Figure ?? . COFFEE analyzes the input problem and decides what variants it is worth testing, as described later. It then provides the autotuner with all of the possible variants, in the form of abstract syntax trees. The autotuner is a template-based code generator. By inspecting an abstract syntax tree, it determines how to generate “wrapping” code that, repeatedly in a *while* loop executed a pre-established amount of time (order of milliseconds), 1) initializes kernel’s input variables with fictitious values and 2) calls the kernel. At the exit of the *while* loop, the times the kernel was invoked is recorded. Eventually, the variant executing the largest number of iterations is designated as the fastest implementation. Suitable compiler directives are used to prevent inlining of all function calls: this avoids the situation in which some variants are inlined and some are not, which would fake the autotuner’s output.

The autotuning process is dynamic: depending on the complexity of the input problem, more or less variants are tried. General heuristics, which can be considered a revisited version of those presented in [Shin et al. 2010], are applied

- Loop permutations that are likely to worsen the performance are excluded from the search space. According to the cost model, and for the same reasons explained in [Luporini et al. 2014], we enable only variants in which the loop over quadrature points is either the outermost or the innermost. This is due to the fact that versions of the code in which such loop lies between the test and trial functions loops are typically lower performing.
- The unroll factors must divide the loop bounds evenly to avoid the introduction of remainder (scalar) loops.
- The innermost loop is never explicitly unrolled. This is because we expect auto-vectorization along this loop, so memory accesses should be kept unit-stride.

Also, the following heuristics, which capture properties of our computational domain, are used

- When both test and trial functions derive from the same function space, the lengths of their corresponding loops are identical. In this case, since for the employed storage layout the memory accesses are symmetrical along these two loops, their interchange is pruned from the search space.

- In general, if relatively high polynomial orders are employed, the loop nest is larger. In these cases, in order to avoid testing too many unroll factors, we impose a bound  $X$  on the loop nest's overall unroll factor, which we found empirically. For example, the sum of the unroll factors of all outer loops cannot exceed  $X$ .
- On the other hand, if the polynomial order is low, i.e. for smaller loop nests, we prune variants that we know will be low-performing, e.g. those resorting to BLAS.
- We select two levels of expression rewriting. In the “base” level, generalized loop-invariant code motion only is applied. This means that only a subset of the rewrite rules exposed in 4 are applicable. In the “aggressive” level, all of the rewrite rules are applied.
- For the expression splitting optimization described in [Luporini et al. 2014] and summarized in Section 2.2, we test only three split factors, namely 1, 2, 4. Also, if the input problem uses mixed function spaces, the iteration space is already split by the Expression Rewriter to avoid computation over zero-columns; in these cases, we do not further apply expression splitting.
- Based on the cost model, the padding and data alignment optimization is always applied.

## 5. PERFORMANCE EVALUATION

### 5.1. Experimental Setup

Experiments were run on a single core of an Intel architecture, a Sandy Bridge I7-2600 CPU, running at 3.4GHz, 32KB L1 cache and 256KB L2 cache. The Intel icc 14.2 compiler was used. The compilation flags used were -O3, -xHost, -xAVX, -ip.

...TODO... Problems chosen...

...TODO... We don't compare to tensor contraction by transitivity on olegaards work

### 5.2. Results for Forms of Increasing Complexity

In Figure 6, ...

In Figure 7, ...

## 6. CONCLUSIONS

We have presented ...

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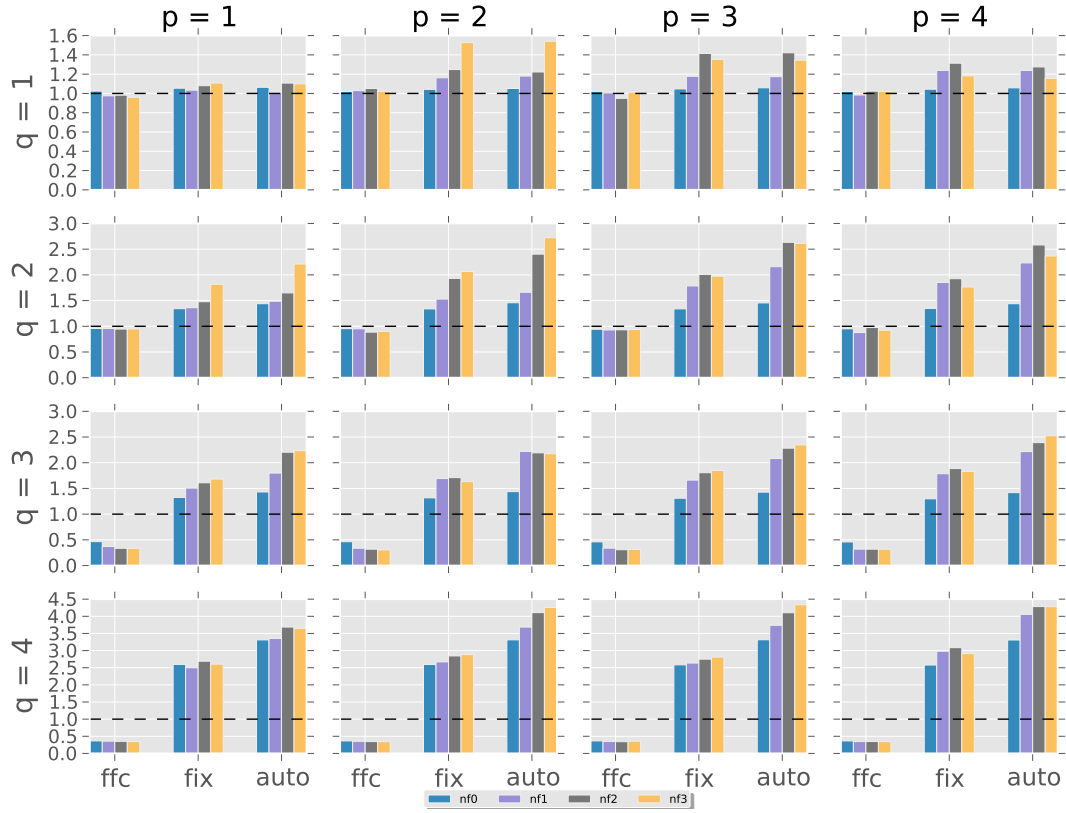


Fig. 6: Helmholtz results.

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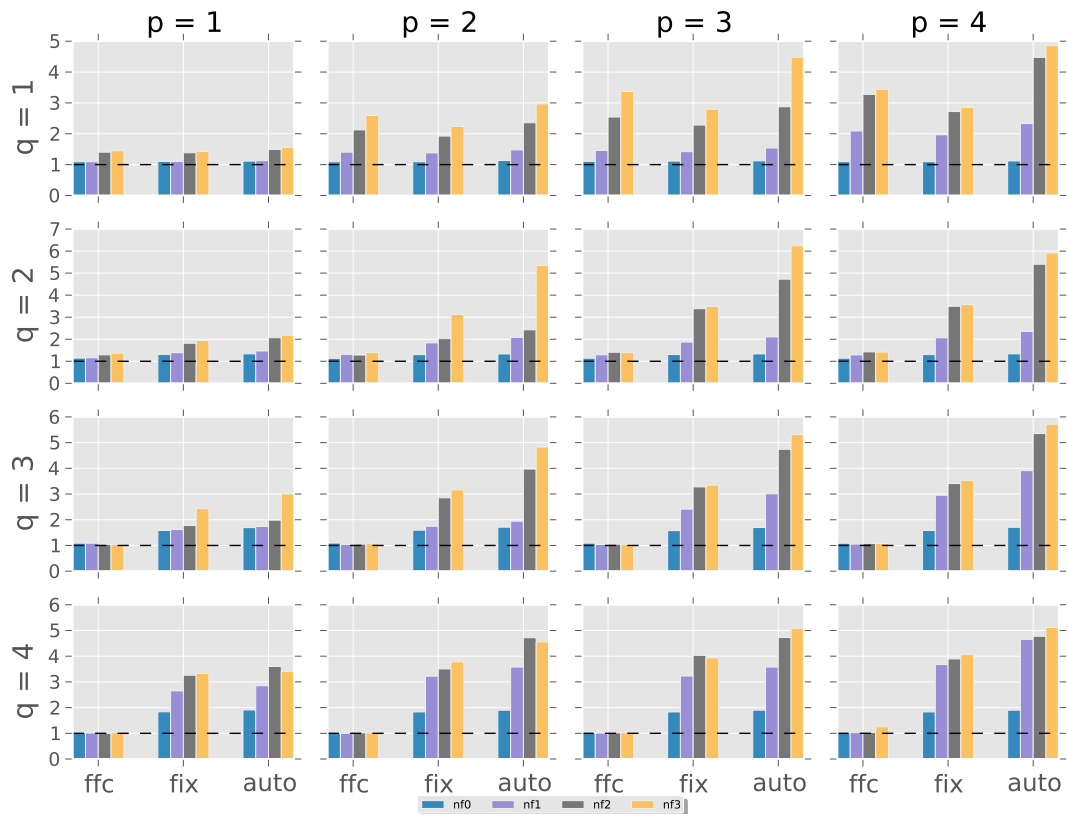


Fig. 7: Elasticity results.