Efficient Evaluation of Arbitrary Box-Splines

This brief report aims to study the differences in runtime performance of box-spline evaluation codes. Different problem sizes and compilers are used to isolate the effects of varying memory management styles across three different Fortran implementations of arbitrary box-spline evaluation.

Box-Spline Definitions

A box spline in $\mathbb{R}^s$ is defined by its *direction vector set* A, composed of n s-vectors where $n \geq s$. Further, A will be written as a $s \times n$ matrix. The first m column vectors of A are denoted by A_m, $m \leq n$. A_s is required to be nonsingular. Consider the unit cube in n dimensions $Q_n = [0, 1)^n$. $A_n(Q_n)$ is now the image (in s dimensions) of Q_n under the linear map A. This image is the region of support for the box spline defined by A_n in s dimensions. The box spline function in s dimensions for A_s is defined as

$$B(x \mid A_s) = \begin{cases} (\det(A_s))^{-1}, & x \in A_s(Q_s), \\ 0, & \text{otherwise.} \end{cases}$$

For A_n when $n > s$ the box spline is computed as

$$B(x \mid A_n) = \int_0^1 B(x - tv_n \mid A_{n-1})dt,$$

where v_n is the nth direction vector of A.

Evaluating Arbitrary Box-Splines

The naive recursive implementation of a box-spline evaluation algorithm is straight forward to implement and has a computational complexity of

$$\mathcal{O}\left(2^{n-s}\frac{n!}{s!}\right),$$

however a naive implementation suffers from numerical instability near the boundaries of the polynomial pieces that compose a box-spline [1]. The numerical instability near boundaries of polynomial pieces can be avoided through postponing the translation of points by direction vectors [2]. A numerically consistent implementation written in *Matlab* is provided by [2]. The computational complexity is reduced to $\mathcal{O}\left(2k^{n-s}\right)$, where k is the number of *unique* direction vectors. [2] also attempts to reduce redundant computations by precomputing all normal vectors defining the boundaries of polynomial pieces with a memory complexity of $\mathcal{O}\left(2^k\right)$.

A *Fortran* implementation of the numerically consistent arbitrary box-spline algorithm is considered here. This implementation does not precompute normal vectors, reducing the memory complexity to $\mathcal{O}\left(sk(n-k)\right)$. An analysis of three different Fortran implementations follows.

Experiment Setup

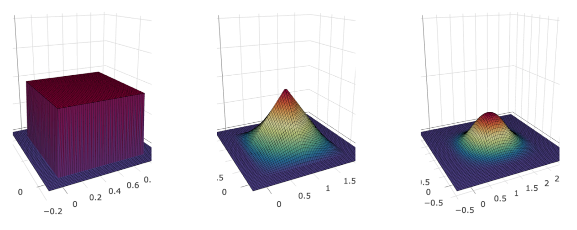
Nearly all combinations of the following variables are considered.

Variable	Values
Element	*TenP*, *Cour*, *ZP*
Number of Evaluation Points	1, 2K, 4K
Element Multiplicity	1, 2, 3, 4, 5
Compiler (Computer)	gfortran (Navajo), sun95 (Navajo), ifort (Pima)
Optimization Flag	None, O2, O3, Os
Box-Spine Version	dynamic, automatic, allocate

Each test is repeated 20 times to capture a corresponding distribution of expected evaluation time. The Fortran intrinsic function *CPU_TIME* is used to time the evaluation of each box-spline. In total 21,600 experiments were conducted. The variable *element* refers to the following two-dimensional direction vector sets with associated multiplicities listed as exponents.

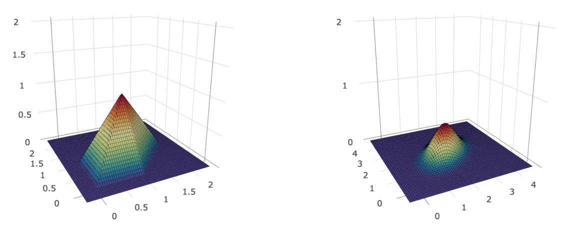
TENSOR PRODUCT B-SPLINE (TENP)

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}^{(1,2,3,4,5)}$$



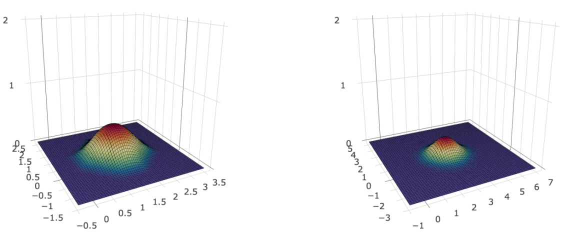
COURANT ELEMENT (COUR)

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}^{(1,2,3)}$$



ZWART-POWELL (ZP)

$$\begin{pmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & -1 & 1 \end{pmatrix}^{(1,2)}$$



Different Box-Spline Implementations

DYNAMIC

Memory allocation is mostly local to subroutines, dynamic allocation is required in order for subroutines to construct their own work arrays of appropriate size.

ALLOCATE

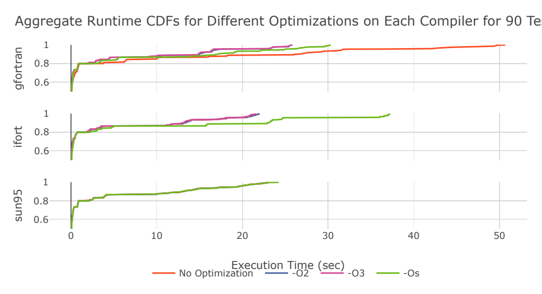
Memory allocation is entirely performed (with the exception of constants) during the top-level entry routine *BOXSPLEV*. No internal routines allocate their own memory, rather they use appropriate slices of initially allocated memory. All allocation sizes are computed at runtime and allocation is performed with the *ALLOCATE* intrinsic.

AUTOMATIC

Same as "Allocate", but all of the allocation sizes are expressed in terms of input arrays and are automatically allocated upon entering the top-level subroutine *BOXSPLEV*.

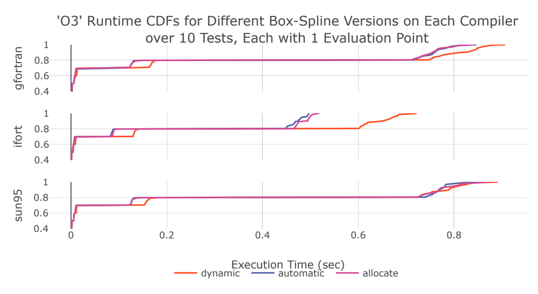
Aggregate Results

First, let's consider the selection of which optimization flag to use when evaluating box-splines. The plot below depicts the aggregate CDFs of all experiment runtimes broken down by compiler and optimization flag.

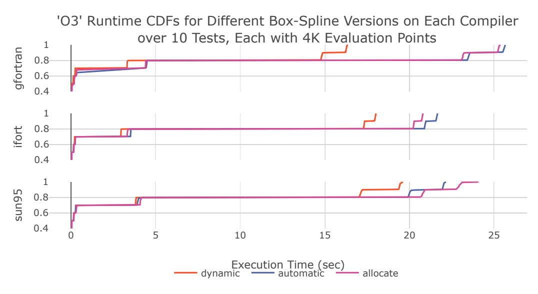


Note that the Sun compiler does not appear to be affected by (cannot find?) differing optimization levels. The GNU compiler suffers the worst performance under no optimization. Generally, O3 appears to provide reasonably good (or the best) performance for both *ifort* and *gfortran*.

Next we consider the performance of the three different box-spline codes using the best optimization on single point evaluation and evaluation at a large number of points.



For single-point evaluation, the *automatic* allocation scheme with the *ifort* compiler produces results most quickly. The dynamic allocation scheme takes more time likely due to the dominating effect of subroutine calls (and allocations) during computation. This effect will likely be observed for any number of points small enough to fit into cache ($< 2^{10}$).



For the most compute-intense experiments, Zwart-Powell multiplicity 2, Courant multiplicity 3 with 4K points, the *dynamic* allocation scheme with the *gfortran* compiler provides the best results. The global allocation scheme takes more time for all compilers when there are enough points to fill cache ($> 2^{10}$).

A NOTE

The *automatic* and *allocate* codes took advantage of a few extra optimizations (other than memory management) not had by *dynamic*. Pending the future use of the *dynamic* framework, those extra optimizations can be included to improve single-point evaluation performance.

Profiling Results

In addition to the large batch test, *gprof* was used to analyze the performance of the *dynamic gfortran* code as well as the *allocate gfortran* code.

Table Legend

The upcoming tables have the following columns.

time (%) — the percentage of the total running time of the program used by this function.

cumulative seconds — a running sum of the number of seconds accounted for by this function and those listed above it.

self seconds — the number of seconds accounted for by this function alone. This is the major sort for this listing.

calls — the number of times this function was invoked, if this function is profiled, else blank.

self ms/call — the average number of milliseconds spent in this function per call, if this function is profiled, else blank.

total ms/call — the average number of milliseconds spent in this function and its descendents per call, if this function is profiled, else blank.

name — the name of the function. This is the minor sort for this listing.

FLAT PROFILE FOR DYNAMIC ALLOCATE (ZP ELEMENT, MULTIPLICITY 2, 1 POINT)

time (%)	cumulative seconds	self seconds	calls	self ms/call	total ms/call	name
40.01	0.06	0.06	1	60.01	150.03	evaluate_box_spline
26.67	0.10	0.04	249032	0.00	0.00	nonzero
20.00	0.13	0.03	69120	0.00	0.00	matrix_det
13.34	0.15	0.02	138240	0.00	0.00	matrix_orthogonal
0.00	0.15	0.00	41672	0.00	0.00	matrix_rank
0.00	0.15	0.00	30153	0.00	0.00	matrix_minimum_norm
0.00	0.15	0.00	1	0.00	0.00	allocate_max_lapack_work
0.00	0.15	0.00	1	0.00	150.03	boxsplev
0.00	0.15	0.00	1	0.00	0.00	matrix_condition_inv

FLAT PROFILE FOR MANUAL ALLOCATE (ZP ELEMENT, MULTIPLICITY 2, 1 POINT)

time (%)	cumulative seconds	self seconds	calls	self ms/call	total ms/call	name
60.01	0.09	0.09	1	90.01	150.02	evaluate_box_spline
26.67	0.13	0.04	110792	0.00	0.00	pack_dvecs
6.67	0.14	0.01	138240	0.00	0.00	compute_orthogonal
6.67	0.15	0.01	69120	0.00	0.00	matrix_det
0.00	0.15	0.00	41672	0.00	0.00	matrix_rank
0.00	0.15	0.00	30153	0.00	0.00	make_dvecs_min_norm
0.00	0.15	0.00	1	0.00	150.02	boxsplev
0.00	0.15	0.00	1	0.00	0.00	matrix_condition_inv
0.00	0.15	0.00	1	0.00	0.00	reserve_memory

The two tables above show that roughly ~25% of the evaluation time is spent managing memory (subroutines *NONZERO* and *PACK_DVECS* have similar function). Notice how that behavior changes once there are 4000 points instead of 1, see below.

FLAT PROFILE FOR DYNAMIC ALLOCATE (ZP ELEMENT, MULTIPLICITY 2, 4K POINTS)

time (%)	cumulative seconds	self seconds	calls	self ms/call	total ms/call	name
99.53	22.16	22.16	1	22.16	22.27	evaluate_box_spline
0.22	22.21	0.05	249032	0.00	0.00	nonzero
0.13	22.24	0.03	138240	0.00	0.00	matrix_orthogonal
0.09	22.26	0.02	41672	0.00	0.00	matrix_rank
0.04	22.27	0.01	69120	0.00	0.00	matrix_det
0.00	22.27	0.00	30153	0.00	0.00	matrix_minimum_norm
0.00	22.27	0.00	1	0.00	0.00	allocate_max_lapack_work
0.00	22.27	0.00	1	0.00	22.27	boxsplev
0.00	22.27	0.00	1	0.00	0.00	matrix_condition_inv

FLAT PROFILE FOR MANUAL ALLOCATE (ZP ELEMENT, MULTIPLICITY 2, 4K POINTS)

time (%)	cumulative seconds	self seconds	calls	self ms/call	total ms/call	name
99.86	31.04	31.04	1	31.04	31.09	evaluate_box_spline
0.10	31.07	0.03	138240	0.00	0.00	compute_orthogonal
0.03	31.08	0.01	110792	0.00	0.00	pack_dvecs
0.03	31.09	0.01	30153	0.00	0.00	make_dvecs_min_norm
0.00	31.09	0.00	69120	0.00	0.00	matrix_det
0.00	31.09	0.00	41672	0.00	0.00	matrix_rank
0.00	31.09	0.00	1	0.00	31.09	boxsplev
0.00	31.09	0.00	1	0.00	0.00	matrix_condition_inv
0.00	31.09	0.00	1	0.00	0.00	reserve_memory

These two tables show that the vast majority of computation time is spent within the *EVALUATE_BOX_SPLINE* routine computing the base case (majority) and processing the results in the non base cases (minority).

References

1. **On the evaluation of box splines**
   de Boor, C., 1993. Numerical Algorithms, Vol 5(1), pp. 5—23. Springer.
2. **Stable evaluation of box-splines**
   Kobbelt, L., 1997. Numerical Algorithms, Vol 14(4), pp. 377—382. Springer.