Inline Vector Compression for Computational Physics

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Abstract

A novel inline data compression method is presented for single-precision vectors in three dimensions. The primary application of the method is for accelerating computational physics calculations where the throughput is bound by memory bandwidth. The scheme employs spherical polar coordinates, angle quantisation, and a bespoke floating-point representation of the magnitude to achieve a fixed compression ratio of 1.5. The anisotropy of this method is considered, along with companding and fractional splitting techniques to improve the efficiency of the representation. We evaluate the scheme numerically within the context of high-order computational fluid-dynamics. For both the isentropic convecting vortex and the Taylor–Green vortex test cases the results are found to be comparable to those without compression. Performance is evaluated for a vector addition kernel on an NVIDIA Titan V GPU; it is demonstrated that a speedup of 1.5 can be achieved.

Keywords: Vector Compression, GPU computing, Flux Reconstruction

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1. Introduction

Over the past 30 years, improvements in computing capabilities, measured in floating-point operations per second, have consistently outpaced improve-
ments in memory bandwidth [1]. A consequence of this is that many numerical methods for partial differential equations are memory bandwidth bound algorithms. Additionally, over the past 10 years, there has been a trend towards the use of graphics processing units (GPUs) for simulation. These accelerators have increased compute and memory bandwidth compared to CPUs. However, one limitation is that the total amount of memory is substantially less than what would accompany an equivalently capable CPU. To this end, there is substantial interest in techniques that can conserve either memory or memory bandwidth.

Arguably the simplest technique is to migrate the numerical scheme from eight-byte double-precision numbers to four-byte single-precision numbers. Such migration has the potential to halve the bandwidth and storage requirements for a code. The feasibility of this depends heavily on both the numerical scheme and its application area. Studies indicate that single-precision arithmetic may be appropriate in computational geosciences, molecular dynamics, and implicit large eddy simulation [2, 3, 4, 5]. More recently, driven primarily by the requirements of the machine learning community, hardware vendors have started to include support for two-byte half-precision arithmetic [6]. However, the restricted range of half-precision floating-point numbers [7] renders them unsuitable for general-purpose computation.

Another promising approach is that of in-line data compression. This takes advantage of the fact that the data in scientific simulations often exhibits spatial correlations and is hence amenable to compression. When evaluating compression schemes in the context of scientific computing, there are several factors to consider. The first is whether the scheme lossless or lossy. Next is the extent to which the scheme admits random access to the compressed data. A third factor is the degree of asymmetry, if any, between the cost of compression and that of decompression. For schemes that are lossy, a fourth factor to consider is if the compression ratio is fixed or variable. Additionally, with lossy schemes, a further consideration is the ability to bound the magnitude of any loss.

A variety of compression schemes, both general purpose, and domain-specific have been proposed. When considering lossless compression, it follows from the Pigeonhole principle that no scheme can guarantee to reduce the size of an input. An immediate consequence of this is that the compression ratio of a lossless scheme must always be a function of the input. A corollary of this is that the maximum problem size in which a code employing lossless in-line compression can robustly handle is identical to that of the
same code without compression. Moreover, the variability in the compression ratio makes it difficult to predict the run-time performance of such a code. As such, within the context of in-line compression for scientific codes, lossy schemes are preferable.

The primary advantage of lossy compression schemes is that not only can higher compression ratios be obtained, but they may admit a fixed compression ratio. Some early work on block data compression was aimed at computer graphics and was based on Vector Quantisation (VQ) [8, 9, 10]. A prominent methodology within VQ is the LBG approach of Linde et al. [11]. This approach used a compression codebook learned *a priori* through optimisation. This allows for efficient vector decompression with a low error when the vector domain is similar to the learned codebook sub-domain. Subsequent methods that have evolved from this include the S3TC method [12], which operates on textures consisting of several pixels. These techniques typically have a large asymmetry between compression and decompression, with compression being orders of magnitude slower. An additional method of importance is the adaptation of LBG by Schneider et al. [13], which employed a codebook initialisation method using principal component analysis based splitting.

More recently, the ZFP algorithm and library were developed [14] to work across small blocks ($4^d$ in size, where $d$ is the dimensionality) with user-controlled fixed-rate compression. This method allowed for independent block access and boasted near symmetric compression and decompression. However, due to the larger block size, this is inappropriate for our desired unstructured application. An algorithm more closely related to the issue of memory-bound compute is the BLOSC methodology and library [15]. BLOSC utilises several compression techniques, including DEFLATE and related methods as well as LZ compression [16, 17]. LZ compression is designed for compression of sequential data-sets, and as a consequence, BLOSC is highly efficient for bandwidth limited calculations with sequential or blocked data access. Yet, similar to ZFP, these techniques are not well suited to the unstructured data access we are concerned with.

Evidently, if compression is to improve the performance of a numerical scheme, a baseline requirement is that the decompression rate must exceed memory bandwidth. An associated requirement is that compression and decompression have comparable costs. This is to enable the compression of dynamic data; that is to say, the output generated by kernels rather than just constant inputs. A tertiary requirement, albeit one which is parti-
larly relevant for numerical schemes on unstructured grids, is for there to be little to no penalty associated with random access to data. Finally, it is desired that the multiple applications of compression/decompression to the same data should not result in substantially different data, i.e. the compression/decompression operator should be idempotent or near-idempotent.

A more applicable set of techniques arises from the compression of individual three-component pixel data. A review of some techniques in this area was presented by Cigolle et al. [18]. It has also been shown by Meyer et al. [19] that 51-bits is sufficient to losslessly represent unit vectors formed of three 32-bit floating-point numbers. Some more recent work presented by Smith et al. [20] looked to apply lossy compression to this case with increased efficiency. The approach taken quantised 3D unit vectors by initially transforming them into spherical coordinates, and subsequently discretising the two angles in bins. These bins were dynamically produced and were dependent on the angle and the desired error level. Hence, the memory overhead, in this case, was reduced from 96-bits to between eight and 30-bits depending on the desired error. This may lead to increased compression ratios, but the additional workload of dynamically calculating the range as well as the resulting unaligned data are deemed to be undesirable to our application. In this paper, we propose a compression scheme for the compression of triplets of single-precision numbers which occur frequently in computational physics. This method extends the work of Smith et al. [20] to 3D vectors of arbitrary length. These techniques allow for unstructured data access and in-line compression and decompression, with approximate symmetry in compression/decompression times.

The remainder of this paper is structured as follows. In Section 2, we outline our compression scheme and analyse its numerical properties through a series of synthetic benchmarks. In Section 4, we implement our scheme into a high-order computational fluid dynamics code and assess its impact on accuracy. Here the performance of our approach on an NVIDIA V100 GPU is evaluated. Finally, the conclusions are discussed in Section 6.
2. Methodology

2.1. Basic Compression Methodology

Given a vector \( \mathbf{x} = [x, y, z]^T \), we begin by writing the transformation from Cartesian to spherical polar coordinates as

\[
\mathbf{x} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} r \cos \theta \sin \phi \\ r \sin \theta \sin \phi \\ r \cos \phi \end{bmatrix},
\]

where \( r, \theta \) and \( \phi \) are defined as

\[
r = \| \mathbf{x} \|_2, \\
\theta = \arctan\left( \frac{y}{x} \right), \\
\phi = \arccos\left( \frac{z}{r} \right).
\]

Here \( \phi \in [0, \pi) \) and \( \theta \in [-\pi, \pi) \). We note here that both of these ranges are substantially smaller than those which can be represented by a 32-bit floating-point number. As a starting point, we consider discretising these angles by representing them as a pair of integers according to

\[
n_\theta = \text{nint}\left( \frac{n_{\theta \text{ max}} (\theta + \pi)}{2\pi} \right) \quad \text{and} \quad n_\phi = \text{nint}\left( \frac{n_{\phi \text{ max}} \phi}{\pi} \right),
\]

where \( n_{\theta \text{ max}} \) and \( n_{\phi \text{ max}} \) are defined as the maximum values supported by the integral type used to store \( \theta \) and \( \phi \), respectively. The function \( \text{nint}(x) \) is defined as that which rounds \( x \) to the nearest integer as per

\[
\text{nint}(x) = \left\lceil \frac{\lfloor 2x \rfloor}{2} \right\rceil,
\]

where we have adopted the round half up tie-breaking rule. The corresponding inverse mappings are

\[
\hat{\theta} = \pi \left( \frac{2n_\theta}{n_{\theta \text{ max}}} - 1 \right) \quad \text{and} \quad \hat{\phi} = \left( \frac{\pi n_\phi}{n_{\phi \text{ max}}} \right).
\]

Here the hat is used to represent a reconstructed angle. The associated absolute errors are then given according to

\[
\theta = \hat{\theta} + \epsilon_\theta + \eta_\theta \quad \text{and} \quad \phi = \hat{\phi} + \epsilon_\phi + \eta_\phi,
\]
where $\epsilon$ is a quantisation error and $\eta$ an arithmetic error. To proceed we shall assume that it is possible to implement the aforementioned compression procedure in a numerically stable manner such the arithmetic error is insignificant compared to the quantisation error. This point shall be explored in Section 3. From the definitions of $\theta$ and $\phi$ it is clear that

$$\epsilon_\theta \in \frac{\pi}{n_{\theta \max}} [-1, 1] \quad \text{and} \quad \epsilon_\phi \in \frac{1}{2} \frac{\pi}{n_{\phi \max}} [-1, 1].$$

(7)

The quantisation errors on $\theta$ and $\phi$ then give rise to a reconstructed vector $\hat{x} = [\hat{x}, \hat{y}, \hat{z}]^T$ with:

$$\hat{x} = r \cos (\theta + \epsilon_\theta) \sin (\phi + \epsilon_\phi),$$

(8a)

$$\hat{y} = r \sin (\theta + \epsilon_\theta) \sin (\phi + \epsilon_\phi),$$

(8b)

$$\hat{z} = r \cos (\phi + \epsilon_\phi).$$

(8c)

Let us define then error vector as $[\epsilon_x, \epsilon_y, \epsilon_z]^T = \hat{x} - x$. Applying the trigonometric sum-to-product identities and assuming $(|\epsilon_\theta|, |\epsilon_\phi|) \ll 1$ we find

$$\epsilon_x \approx r (\epsilon_\phi \cos \theta \cos \phi - \epsilon_\theta \sin \theta \sin \phi),$$

(9a)

$$\epsilon_y \approx r (\epsilon_\phi \sin \theta \cos \phi + \epsilon_\theta \cos \theta \sin \phi),$$

(9b)

$$\epsilon_z \approx r \epsilon_\phi \sin \phi.$$  

(9c)

2.2. Base Scheme Evaluation

We now wish to evaluate the error of the base method by which we mean discretising $n_\theta$ and $n_\phi$ with 16-bits and storing the magnitude as a standard single-precision floating-point (SPFP). This evaluation was performed by randomly sampling $\theta$ and $\phi$ such that the cartesian points are uniformly distributed over a unit sphere. This, together with the computation of $x$, is carried out using double-precision floating-point (DPFP) numbers. Then, before $x$ is compressed, the components are converted to SPFP. This was to ensure that all points on the unit ball, in single-precision, could be sampled. To minimise the arithmetic error in the compression and decompression steps all the intermediates real numbers used were cast as DPFP numbers. Then the $L_2$ norm of the error between the SPFP $x$ and the vector after compression and decompression, $\hat{x}$, was calculated. These results can be seen in Fig. 1. Here, the level of anisotropy in the method is clearly visible, with both the error described in Eq. (9) and the larger range of $\theta$ contributing to this.
2.3. Increasing Discretisation Resolution

In Section 2.1, the basic compression methodology was presented and evaluated in Section 2.2. We now wish to investigate if the error magnitude and degree of anisotropy can be reduced while still limiting the result to 64-bits. It is proposed that bits from the vector magnitude may be redistributed to increase the quantisation on the angles. An aspect of this compression technique that should be used to inform bit redistribution is that the range of $\theta$ is twice that of $\phi$. From Eq. (7 & 9), it can be seen that this will impact the error; hence, $\theta$ should be quantised with an additional bit.

The most straightforward bit to repurpose is the sign bit of $r$ since the magnitude will always be positive. Two subsequent techniques will be introduced as a means of recovering further bits from the magnitude. The first method is to remove bits from the exponent of the SPFP number representing $r$. This is motivated by the maximum and minimum values of the exponent being $2^{127} \approx 10^{38}$ and $2^{-126} \approx 10^{-38}$ respectively. This range of values is larger than is typically encountered in the simulation of physical phenomena, and hence it may be possible to reduce the range of the exponent without adversely affecting the results. Such a reduction may be accomplished as follows, beginning by describing the procedure for calculating the exponent [7], $e$

$$e = E_8 - b_8,$$ \hspace{1cm} (10)

where $E_8$ is the 8 bit integer representation of the exponent bits stored in the SPFP number. Furthermore, $b_8$ is a bias that shifts the range of $E_8$ such
that $e$ can take negative values. In the case of SPFP $b_8 = 127$ such that $e \in \{-126, \ldots, 127\}$.

Reducing the exponent length, instead storing $E_7$, will then lead to a reduction in the range of $e$. Therefore, the method is

$$\hat{E}_8 = E_7 + b_8 - b_7,$$

where $b_7$ is a new bias to be set and $\hat{E}_8$ is the reconstructed exponent integer needed for SPFP arithmetic. It can then be seen that this will lead to

$$e = \hat{E}_8 - b_8 = E_7 - b_7,$$

such that

$$-(b_7 + 1) \leq e \leq 2^7 - (b_7 + 2).$$

When removing a single bit from the exponent it was hypothesised that $b_7 = 80$ was a reasonable compromise for computational fluids calculations. An asymmetric bias was chosen based on the hypothesis that, often in physical simulations, small numbers and zeros are important in the phenomena exhibited. Conversely, very large numbers in properly normalised calculations are typically indicative of a diverging solution and hence limiting the range here is deemed reasonable. However, the degree of exponent compression and bias could be varied on a case-by-case basis.

Going further, we will now consider how bits may be removed from the mantissa. Starting from SPFP numbers [7], the mantissa, $T$, or the fraction, is defined using 24-bits as:

$$T_{24} = d_0.d_1 \cdots d_{22}d_{23} = 1.d_1 \cdots d_{22}d_{23},$$

where, through proper normalisation, $d_0$ is assumed to always be 1 and hence only 23 bits are stored. Bits may then be removed from the tail of the mantissa and repurposed. Taking the example of removing one bit, $d_{23}$, and replacing it by zero in the reconstructed mantissa we get

$$\hat{T}_{24} = 1.d_1 \cdots d_{22}.$$

Within the set of SPFP numbers there is a subset called normal numbers. This is the case when the bit $d_0$ is always 1, i.e. the binary point of the mantissa is shifted such that the $d_0 = 1$. To normalise the number, the binary point is moved by increasing or decreasing the exponent. In the case
of SPFP, if the exponent, $E_8$, equals 1 and $d_0 \neq 1$ then the number is said to be subnormal. The handling of this exception is usually done by the hardware based on the compiler options. However, with $E_7$ this has to be handled by the compression algorithm. Hence, we impose that subnormal numbers, i.e. when $E_7 = 1$, are set to the lowest supported value.

Throughout the remainder of this work we will use the following notation to describe how the 64 bits are used: $\langle s, e, m \rangle - p - t$, where $s$ indicates the presence of a sign bit; $e$ is the number of exponent bits; $m$ is the number of mantissa bits; and $p$ and $t$ are the number of bits in $n_\phi$ and $n_\theta$ respectively. Some potential bit layouts are shown in Fig. 2 which are investigated later.

![Diagram of bit layouts](image)

Figure 2: Compression regimes under consideration.

We will now compare the error on the unit ball of three different bit distributions: $\langle 0, 8, 23 \rangle$-16-17, $\langle 0, 7, 23 \rangle$-17-17, and $\langle 0, 7, 22 \rangle$-17-18. The methodology followed here is the same as in Section 2.1. The impact of bit utilisation on the error is shown in Fig. 3. It is clear that, not only are all three methods an improvement over the base scheme shown in Fig. 1, but that the additional angle resolution has a significant impact on the error. In this instance, the average error over the samples was found to be $1.55 \times 10^{-5}$, $1.07 \times 10^{-5}$, and $7.74 \times 10^{-6}$, respectively.

A further investigation was performed where the average error was calculated while varying the ball radius in $\left[10^{-8}, 10^8\right]$. It was found that the
Figure 3: Error of random vector field on unit ball for $10^8$ samples.
average error, normalised by the radius, was approximately constant. Therefore, in this range, the exponent and mantissa contraction has not led to any additional dependence of error on $r$.

### 2.4. Fractional Splitting

The schemes so far described have discretised the angles using powers of two due to their connection to binary representation. For example, $n_{\phi,\text{max}} = 2^{16} - 1$, $n_{\theta,\text{max}} = 2^{17} - 1$. It is proposed that it may be possible to split the available discretisation at some other interface. This can be defined in the general form for some number $n_p$, where the total number of bit available is $p$, and $n_{\phi}$ and $n_{\theta}$ are encoded based on:

\begin{align}
    n_p &= n_{\phi}(n_{\theta,\text{max}} + 1) + n_{\theta}, \quad (15a) \\
    n_{p,\text{max}} &= (n_{\phi,\text{max}} + 1)(n_{\theta,\text{max}} + 1) - 1 < 2^p. \quad (15b)
\end{align}

For the case of $p = 35$, where the additional bits have been obtained through a reduction in the exponent range and mantissa precision, we will vary $n_{\phi,\text{max}} + 1 \in [2^{16}, \ldots, 2^{18}]$. By setting $n_{\phi,\text{max}}$, Eq. (15) then constrains $n_{\theta,\text{max}}$. For each of the splitting chosen we will then calculate the mean and standard sample deviation of the error on the unit ball, as defined by

\begin{align}
    e_i &= \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|_2, \quad \bar{e} = \frac{1}{N} \sum_{i=1}^{N} e_i, \quad \sigma(e)^2 = \frac{1}{N-1} \sum_{i=1}^{N} (e_i - \bar{e})^2. \quad (16)
\end{align}

As evident from Fig. 4, variation of the splitting location from $n_{\phi,\text{max}} = 2^{17}$ has only a minor impact on the error exhibited by the compression method. Hence, as the reduction in $\sigma$ that can be achieved is small and as fractional splitting would increase code complexity, it is deemed to be of insufficient benefit to be used.

### 2.5. Angle Discretisation Companding

Equation (9), together with Eq. (7), made clear that a uniform discretisation will give rise to anisotropy in this compression method. We will now discuss some alternative discretisation methods with the aim of reducing this anisotropy. Firstly, for an angle discretisation to be practical it must be easily invertible, for example Eq. (3) is straightforwardly inverted as in Eq. (5). Therefore, we can straightforwardly use any transformation where $n = \text{nint} f(\psi)$ and $\hat{\psi} = f^{-1}(n)$ are computable in finite time. This does
however severely limit the possibly to functions implemented—together with their inverse—by compilers. For example, \( n_{\max} f(\psi) = \psi \) is admissible but \( n_{\max} f(\psi) = \psi + \sin(4\pi \psi)/4\pi \) is not. This latter example was chosen as, from the previous error analysis, it can be thought to be a good candidate to reduce the error. However, to invert the discretisation, a root finding method, such as the fixed point iteration, has to be used. This is due to the stationary points in the mapping which can lead to large inaccuracies when a high degree of angle discretisation was used. That leads us to the question that, if stationary points could be avoided, could it be permissible to use a mapping that is not simply inverted? At the present time it is believed that it may be possible, but the root finding method is likely to be computationally expensive, especially to the desired level of precision, which in this case is close to machine precision.

Smith et al. [20] proposed a method where the number of bins used for \( \theta \) was varied based on an error tolerance, \( \tau \), and the value of \( \phi \) that would remove anisotropy. This was defined as

\[
\frac{1}{\hat{n}_{\theta,\max}} = \cos^{-1}\left(\frac{\cos \tau - \cos \phi \cos \left(\phi + \frac{\pi}{2n_{\phi,\max}}\right)}{\sin \phi \sin \left(\phi + \frac{\pi}{2n_{\phi,\max}}\right)}\right), \tag{17a}
\]

\[
n_{\theta,\max} = \lceil \pi \hat{n}_{\theta,\max} \rceil. \tag{17b}
\]

From this definition it should be clear that this poses a high computa-
tional cost for both compression and decompression, due to several trigono-
metric function evaluations, each of which can run to hundreds of clock cycles. Furthermore, it can be shown that for this relationship, the maximum num-
ber of bins as the tolerance tends to zero is equal to $2n_{\phi,max}$, which in turn
means that this method achieves isotropy by removing $\theta$ bins as $\phi \to \pi/2$. Therefore, resolution will be wasted when fixed rate compression is used.
Hence, this method is deemed unsuitable for the application proposed here.

Two alternative invertible mappings were tested. The first was $n = \text{nint}(n_{\text{max}}(1 - \cos \psi)/2)$, which does contain stationary points, and was found
to give far worse error performance when applied to $\phi$ and $\theta$. A second map-
ingen that was attempted was

$$n = \text{nint} \left( mn_{\text{max}} \left[ \tanh \left( \gamma(2\psi - 1) + c \right) \right] \right), \quad c = \tanh \gamma, \quad m = \frac{1}{2c}. \quad (18)$$

Performance was again measured by the mean and standard deviation of
the error defined in Eq. (16). It was found that $\gamma = 0.5$ could give a reduction in $\sigma(e)$ of $\sim 2\%$ and therefore, it is clear that the additional cost of this
discretisation distribution outweighs the benefit. A final attempt is made
to reduce the anisotropy by optimising the discretisation brackets to reduce $\sigma(e)$. This was initially performed for $n_{\theta,max} = 200$ and $n_{\phi,max} = 100$, with
the error evaluated on a unit sphere at $\sim 3 \times 10^5$ points. The optimisation was
performed using a simulated annealing approach [21] where the cost function
was $\sigma(e)$. In this case the uniform distribution gave $\sigma(e) \approx 7.3 \times 10^{-3}$
and the optimum distribution gave $\sigma(e) \approx 4.8 \times 10^{-3}$. However, the optimal
distribution found was non-smooth, with large variation in bucket width even
when smoothing was applied to perturbations in the optimiser. Hence, such
distributions are not likely to be computationally efficient in reality, due to
the need for a lookup table or other similar device.

3. Implementation

The analysis in the previous sections concluded that the average error
and the absolute level of anisotropy can be reduced significantly when using
a bit layout of $\langle 0, 7, 22 \rangle$-17-18. During these experiments, all intermediate
calculations were performed using double-precision floating-point (DPFP)
arithmetic. This has a clear increase in computational cost and, after char-
acterising the schemes, we wished to move some or all of the calculation to
single-precision. However, through experimentation, differences in the error
were noticed as the implementation of the compression routine was varied slightly. This highlighted that under some circumstances the assumption that arithmetic errors, η, were small is false unless care is taken during implementation of these methods. Here we present an exploration of these variations and demonstrate some of the sensitivities of the compression method to the intermediate working precision. Recommendations will be made based on this investigation as to how the arithmetic error can be kept small when implementing this technique.

In summary of the compression algorithm, three SPFP numbers, x, are passed to a function where θ, φ, and r are calculated according to Eq. (2). Then, θ and φ are quantised and the exponent and mantissa of r are manipulated. Finally, the resulting bits are combined and 64 bits are returned from the function. The effect of manipulating r and the degree of quantisation of θ and φ were explored in Section 2, but the intermediate precision when calculating and quantising θ and φ were not discussed.

When calculating θ or φ there are two clear options: either all intermediates are SPFP or DPFP. For double-precision, this requires that x is converted to double when used, while the single-precision case is more straightforward. To characterise the difference, a similar test to Section 2 was used where points on the unit sphere, S², were sampled and the mean error and maximum error was calculated. The error from points in [-1, 1]³ is also considered and the error is normalised by the vector magnitude before averaging and finding the maximum. Throughout these investigations we have used ⟨0, 7, 22⟩-17-18 compression. The results for a C++ implementation are shown in Table 1.

|         | tan⁻¹    | cos⁻¹    | e   | max (ε) | X     |
|---------|----------|----------|-----|---------|-------|
| Single  | Single   | 8.2832 × 10⁻⁶ | 6.4805 × 10⁻⁵ | S²    |
| Single  | Double   | 8.2828 × 10⁻⁶ | 1.7059 × 10⁻⁵ | S²    |
| Double  | Single   | 8.2831 × 10⁻⁶ | 6.4805 × 10⁻⁵ | S²    |
| Double  | Double   | 8.2827 × 10⁻⁶ | 1.7017 × 10⁻⁵ | S²    |
| Single  | Single   | 8.3016 × 10⁻⁶ | 2.7380 × 10⁻⁴ | [-1, 1]³ |
| Single  | Double   | 8.3013 × 10⁻⁶ | 1.7064 × 10⁻⁵ | [-1, 1]³ |
| Double  | Single   | 8.3014 × 10⁻⁶ | 2.7380 × 10⁻⁴ | [-1, 1]³ |
| Double  | Double   | 8.3012 × 10⁻⁶ | 1.7064 × 10⁻⁵ | [-1, 1]³ |

Table 1: Normalised error for x ∈ X.
Table 1 evidently shows that the error is largely invariant to the intermediate precision of $\tan^{-1}$ used in the $\theta$ calculation. However, the error was found to be susceptible to the intermediate precision of $\phi$, where moving to single-precision caused a significant increase in the error. When calculating $\phi$, $z/r$ is required, which is understood to be the source of the error as division can generate large errors. This error will then propagate through several subsequent steps in the compression routine. Two remedies were considered where DPFP was used for the division and the result was converted to SPFP before use in $\cos^{-1}$, as well as the division in SPFP and $\cos^{-1}$ in double. However, both gave the similar results as entirely SPFP processes. It is concluded that the calculation of $\phi$ should be performed in DPFP but $\theta$ can be performed in SPFP. To further highlight this, the value of $n_{\theta}$ and $n_{\phi}$ calculated in SPFP were compared to using DPFP. Table 2 records the number of misses and it is clear that $\phi$ is significantly more lossy than $\theta$.

Table 2: Single precision bin misses compared to double for $x \in X$.

| $n_{\theta}$ misses | $n_{\phi}$ misses | $X$          |
|---------------------|-------------------|--------------|
| 0.2008%             | 0.2603%           | $X = S^2$    |
| 0.2039%             | 0.2411%           | $X = [-1, 1]^3$ |

The effect of precision on the quantisation of $\theta$ and $\phi$ was also investigated. In the quantisation of $\phi$ it was found that the error and bin misses were invariant with precision. Therefore, after calculating $\phi$ in DPFP, it can be cast to a SPFP number for the quantisation. Similar results were found for $\theta$. A further, albeit small, reduction in the $\theta$ quantisation error was obtained by moving the domain for $\theta$ from $[0, 2\pi]$ to $[-\pi, \pi]$. This avoids the addition, but the minus sign has to be detected and accounted for in the quantisation.

For completeness, these tests were also performed using: CUDA-C, Fortran, and CUDA-Fortran using the same sample points. The results were found to be similar and in the case of the error terms were identical to the third and fourth significant figures. Sample implementations in the respective languages are included in the EMS.

4. Applications to high-order CFD

The computational setting chosen to perform the numerical testing within is the Flux Reconstruction discontinuous spectral element method [22, 23].
This is a high-order method where the domain is decomposed into sub-domains within which polynomials are fitted. We will restrict the computational sub-domains here to be hexahedral, but other topologies are supported within FR. Unless otherwise stated, tests will be carried out at degree $k = 4$. The internal solution point quadrature, as well as the interface flux point quadrature, used will be a tensor product of a Gauss-Legendre quadrature. The inviscid common interface flux is calculated using a Rusanov’s method with Davis wave speeds \[25, 26\]. Furthermore, the common viscous interface flux is set using the BR1 method of Bassi and Rebay \[27\]. The authors are interested in this method due the possibility for efficient porting and use of modern GPU hardware \[1, 28\]. Consequently, at several points this method can suffer from being memory-bandwidth bound.

### 4.1. Isentropic Convecting Vortex

We will begin our numerical experiments with the isentropic convecting vortex (ICV) as defined by Shu \[29\]. This is a solution to the compressible Euler’s equations for an ideal gas, written in 3D as:

$$
\begin{align*}
\frac{\partial Q}{\partial t} + \nabla \cdot F &= 0, \\
Q &= [\rho \quad \rho u \quad \rho v \quad \rho w \quad E]^T, \\
E &= \frac{1}{2} \rho (u^2 + v^2 + w^2) + \frac{p}{\gamma - 1},
\end{align*}
$$

where

$$
F = \begin{bmatrix}
\rho u & \rho v & \rho w \\
\rho u^2 + p & \rho u v & \rho u w \\
\rho u v & \rho v^2 + p & \rho v w \\
\rho u w & \rho v w & \rho w^2 + p \\
u(E + p) & v(E + p) & w(E + p)
\end{bmatrix}.
$$

Here $p$ is the pressure, $E$ is the total energy, and $\gamma$ is the ratio of specific heats. The compression algorithm was then applied on the rows of $F$ and the compressed vectors are highlighted in Eq. (20).
The initial condition for the ICV was taken to be defined as:

\begin{align}
    u &= u_0 + \frac{\beta}{2\pi} (y_0 - y) \exp \left( \frac{1 - r^2}{2} \right), \\
    v &= v_0 - \frac{\beta}{2\pi} (x_0 - x) \exp \left( \frac{1 - r^2}{2} \right), \\
    w &= 0, \\
    p &= \left( 1 - \frac{(\gamma - 1)\beta^2}{8\gamma\pi^2} \exp \left( 1 - r^2 \right) \right)^{\frac{\gamma}{\gamma - 1}}, \\
    \rho &= p^{\frac{1}{\gamma}}, \\
    r &= ||x - x_0||_2,
\end{align}

where \( \beta \) is a constant controlling vortex strength, typically set to \( \beta = 5 \). For the purposes of this test the convective velocities, \( u_0 \) and \( v_0 \), were set such that they vary on the unit circle, as:

\[ u_0 = \cos \psi \quad \text{and} \quad v_0 = \sin \psi. \]

This flow was applied to a fully periodic domain with \( \Omega = [0, 20] \times [0, 20] \times [0, 2], \) which was divided into \( 20 \times 20 \times 2 \) subdomains.
The ICV test case permits the actual solution error to be analytically calculated at later times, and this is the primary advantage of using this test case. Here the results presented will focus on the absolute error in $\rho$ averaged over the whole domain, denoted as $e_1$. Defined as:

$$e_1(t) = \frac{1}{N} \sum_{i=1}^{N} \| \rho_{\text{exact}}(t, x_i) - \rho(t, x_i) \|_1.$$  \hspace{1cm} (23)

Here $N$ is the number of points in used in the average. Here we have averaged over all the solution points in the domain, which for the grid defined is $20 \times 20 \times 2 \times (4 + 1)^3 = 10^5$. The error was considered at $t = 20$, which for $\psi = \{0, 90\}$ should lead to the vortex returning to the start position. The error as the convective velocity angle is varied is displayed in Fig. 6; the line labelled as 'base' is the behaviour for the unaltered scheme running in single precision. Anisotropy of the maximal-order polynomial basis used in this tensor product formulation is clearly visible as a reduction in the error by approximately half as the angle is varied.

![Figure 6: ICV error with flow angle for various methods for degree $k = 4$ FR.](image)

Going on to study the effect of compression, it is clear the additional bits obtained from the sign, exponent, and mantissa, respectively, have had
a significant impact on the error of the scheme, with \(0, 7, 22\)-17-18 having comparative error to the base scheme.

4.2. Taylor Green Vortex

We will now move on to consideration of the more complex compressible Navier–Stokes Equation set, written in the form

\[ Q_t + \nabla \cdot F = \nabla \cdot F^v, \quad \text{where} \]

\[ F^v = \begin{bmatrix}
\tau_{xx} & \tau_{yx} & \tau_{zx} \\
\tau_{xy} & \tau_{yy} & \tau_{zy} \\
\tau_{xz} & \tau_{yz} & \tau_{zz} \\
u \tau_{xx} + \nu \tau_{xy} + \nu \tau_{xz} - q_x & \nu \tau_{yx} + \nu \tau_{yy} + \nu \tau_{yz} - q_y & \nu \tau_{zx} + \nu \tau_{zy} + \nu \tau_{zz} - q_z
\end{bmatrix}. \quad (24a)\]

Here \(\tau_{ij}\) is the standard viscous stress tensor and \(q_i\) are the components of \(\kappa \nabla T\). Setting the bulk viscosity to zero, these may be written as

\[ \tau_{xx} = 2\lambda u_x - \lambda(v_y + w_z), \quad \tau_{yy} = 2\lambda v_y - \lambda(w_z + u_x), \quad \tau_{zz} = 2\lambda w_z - \lambda(u_x + v_y), \quad (25a)\]

\[ \tau_{xy} = \tau_{yx} = \mu(u_y + v_x), \quad \tau_{yz} = \tau_{zy} = \mu(v_z + w_y), \quad \tau_{xz} = \tau_{zx} = \mu(w_x + u_z), \quad (25b)\]

\[ q = [q_1, q_2, q_3]^T = -\kappa \nabla T, \quad (25c)\]

where \(\lambda = 2\mu/3\) and \(\kappa\) is the thermal diffusivity. This equation set, after application to the FR methodology, offers several opportunities for compression. Again the flux terms can compressed, as in Eq. (20), but to aggregate of \(F - F^v\). With compression applied for these flux terms at both the FR solution and flux points. Furthermore, the gradient terms used in the construction of \(\tau_{XX}\) can be compressed, once again at the FR solution and flux points.

The which was applied to the Navier–Stokes equations was the Taylor–Green vortex \[30, 31\], whose initial condition is defined with

\[ u = \begin{bmatrix} U_0 f(x, y, z) \\ -U_0 f(y, x, z) \\ 0 \end{bmatrix}, \quad (26a)\]

\[ p = p(x, y, z). \quad (26b)\]
Here we have defined the functions $f$ and $p$ for simplicity and they take the form:

\[
f(x, y, z) = \sin \left( \frac{x}{k} \right) \cos \left( \frac{y}{k} \right) \cos \left( \frac{z}{k} \right), \tag{27a}
\]
\[
p(x, y, z) = p_0 + \frac{\rho_0 U_0^2}{16} \left( \cos \left( \frac{2x}{k} \right) + \cos \left( \frac{2y}{k} \right) \right) \left( \cos \left( \frac{2z}{k} \right) + 2 \right). \tag{27b}
\]

The density is then set based on Boyle’s Law, assuming an ideal gas,

\[\rho = \frac{p \rho_0}{p_0}.\]

We introduced these functions in the definition of the TGV as it permits clear notation for spatial transformation of the initial condition. With the condition in Eq. (26) being the condition traditionally used.

The compression investigated here was shown in Section 2 to have some degree on anisotropy and hence we also investigated a slight modification of the initial condition

\[
\mathbf{u} = \begin{bmatrix} U_0 f (z, y, x) \\ -U_0 f (y, z, x) \\ 0 \end{bmatrix}, \tag{28a}
\]
\[
p = p(z, y, x). \tag{28b}
\]

This condition exhibits a rotation through $90^\circ$. Evaluation was made through the following dissipation metrics:

\[
\xi_1 = -\frac{1}{\rho_0 U_0^3 |\Omega|} \frac{d}{dt} \int_{\Omega} \frac{1}{2} \rho(x, t) (\mathbf{u} \cdot \mathbf{u}) dx, \tag{29}
\]
\[
\xi_2 = \frac{1}{2 \mu U_0^3 |\Omega|} \int_{\Omega} \frac{1}{2} \rho(x, t) (\mathbf{\omega} \cdot \mathbf{\omega}) dx, \text{ where } \mathbf{\omega} = \nabla \times \mathbf{u}. \tag{30}
\]

Throughout, a TGV was considered for $\Omega = [0, 2\pi]^3$ with $Re = 1600$, $Ma = 0.08$ and $Pr = 0.71$, based on $U_0 = 1$, $k = 1$, $\rho_0 = 1$ and $p_0 = 100$. Furthermore, low-storage explicit four-stage fourth-order Runge–Kutta time integration was used and a time step was chosen such that results were independent of $\Delta t$. For the cases investigated here that meant a value of $\Delta t = 10^{-3}$. Comparative DNS results were obtained from DeBonis [32].
Figure 7: Taylor–Green Vortex enstrophy based decay rate, compression comparison for $Re = 1600$ and $Ma = 0.08$ on a $16^3$ element hexahedral grid with degree $k = 4$ FR.
Initially, comparison is made between the three compression regimens when using the initial condition set out in Eq. (26) and Fig. 7 presents these results. This particular flow is initially laminar and transition to turbulence occurs approximately for $3 < t < 7$. It is clear that compression has had a limited impact on the laminar region, which may have been predicted from the ICV results. Throughout transition though, as turbulent structures have developed small scale motions have increased importance. In particular, the compression method will introduce small perturbations, which can effect the energy at the smallest scales. It can be seen from Fig. 7b that compression has lead to an increase in the peak turbulent dissipation. This may be attributed to the compression error introducing pointwise oscillations which has the effect of energising the highest frequency modes of the scheme. These high frequency modes are known to have high dissipation [33], and hence it is believed this is causing the excess dissipation observed. From the ICV tests, it is known that the compression regime $\langle 0, 7, 22 \rangle -17-18$ is less erroneous. This is concurrent with the theory that the compression error leads to dissipation in this case as the lowest additional dissipation is observed for this compression regime.

As was displayed in Section 2.3, the proposed compression method has some degree of anisotropy. To understand if this anisotropy has a significant impact on the TGV test case the initial condition was transformed to that of Eq. (28). Comparison is displayed in Fig. 8a for the compression regime $\langle 0, 7, 22 \rangle -17-18$. It is clear that anisotropy has affected the results in this case, however the difference is small compared to the potential difference caused by reduction to $\langle 0, 8, 23 \rangle -16-17$. Therefore, the degree of isotropy achieved by $\langle 0, 7, 22 \rangle -17-18$ is deemed to be acceptable.

Finally, within FR there is the potential for compression to be applied to either the flux terms, gradient terms, or both of these components. As gradient terms are solely used in the calculation of the viscous flux, and, as the viscous flux typically has significantly smaller magnitude than the inviscid flux, it is hypothesised that compressing the flux will have a larger impact than the gradient in this case. Figure 8b makes this comparison. Firstly, it may be observed that the differences are of the order of the differences observed in Fig. 7. It seems that compression of both terms leads to smaller observed differences. This could be due to all the terms being in a consistent number space.
Figure 8: Taylor–Green Vortex enstrophy based decay rate, transformed and partial compression comparison for $Re = 1600$ and $Ma = 0.08$ on a $16^3$ element hexahedral grid with degree $k = 4$ FR.
5. Performance Evaluation

We will now consider the computational performance of the compression/decompression method. For this the following problem was considered:

\[ C = A + B, \]  

(31)

where \( A, B, \) and \( C \) are \( 3 \times N \) matrices of single-precision numbers. This case was chosen as the FLOPs required are minimal, and consequently is likely to become memory bandwidth bound. Due to the low number of FLOPs in this calculation, this can be thought of as a worst case scenario and any performance benefit here will likely carry over to dense matrix multiplications.

A kernel was designed that took in two 64-bit unsigned integers and returned one 64-bit unsigned integer. Within the kernel, the inputs were decompressed into two 3D vectors, the vectors were added, and the result was compressed to give the output. Throughout \( 0, 7, 22 \)-17-18 compression was used. Due to the highly parallel nature of the flux reconstruction algorithm, GPUs are particularly effective, and so the tests here were performed on a GPU. In particular, the NVIDIA Titan V was used which has the following properties, found using utilities in the CUDA library.

| Table 3: NVIDIA Titan V Key Statistics. |
|----------------------------------------|
| Global Memory | 12.6 GB |
| L2 Cache | 4.5 MiB |
| Clock Rate | 1.455 GHz |
| Registers/Block | 65536 |

The results comparing the speedup afforded by the kernel incorporating compression as matrix size varies are shown in Fig. 9. Included are lines to indicate the theoretical peak speedup (dashed line), as well as a line indicating the baseline problem size which exceeds the capacity of the L2 cache (dotted line). It is clear that once the matrices may no longer be entirely resident in L2 cache, the compression kernel becomes more favourable. This proves our hypothesis that this form of compression may aid in reducing computation time in applications that are bound by global memory bandwidth. Furthermore, by \( N = 2^{22} \) close to peak speedup is obtained, which is equivalent to 144 MiB of data in the baseline case. 144 MiB is small in global terms and so it may be expected that many kernel could benefit from this compression.
6. Conclusions

A compression algorithm was presented for three-dimensional single-precision vectors that was designed to work on local data to reduce memory bandwidth when retrieving vectors from global memory. The method utilised spherical polar coordinates, discretising the angles using integers, and using a modified floating-point bit layout. It was found that a seven-bit exponent and 22-bit mantissa were sufficient to increase the quantisation of the angles to such a point that in numerical test cases on Euler’s equations, the error was appreciably similar to the baseline scheme. Further tests were performed on the compressible Navier–Stokes equations, particularly the transitional Taylor-Green test case. Only limited variation in results was observed when compression was applied in this case. Lastly, performance evaluation showed that a speedup close to the theoretical peak could be achieved for cases that could not be entirely resident in the L2 cache.

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