Alternatives to IEEE: NextGen Number Formats for Scientific Computing

IPAM Workshop II: HPC and Data Science for Scientific Discovery

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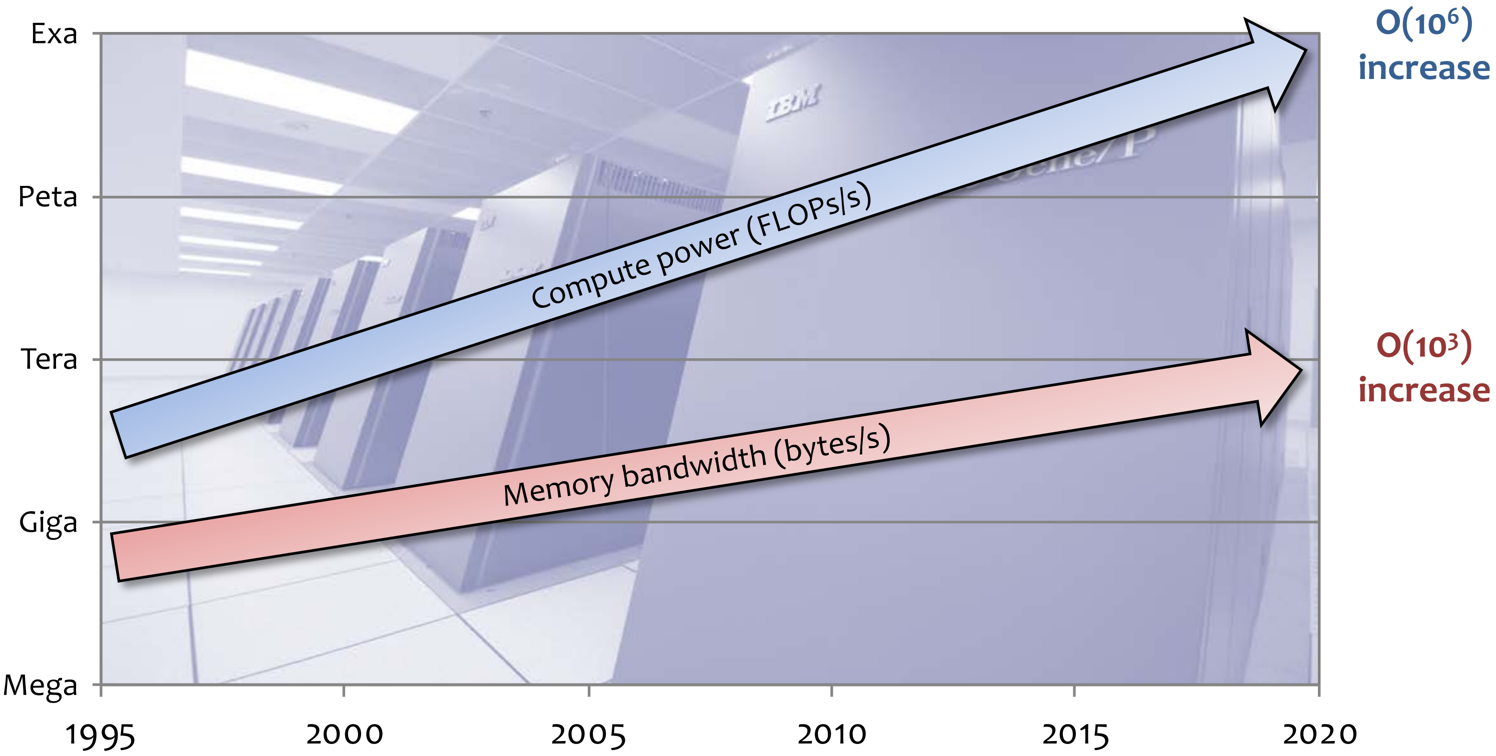
Data movement will dictate performance and power usage at exascale



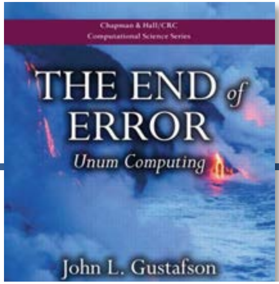
Uneconomical floating types and excessive precision are contributing to data movement

- IEEE assumes "one exponent size fits all"
  - **Insufficient precision** for some computations, e.g. catastrophic cancellation
  - **Insufficient dynamic range** for others, e.g. under- or overflow in exponentials
  - For these reasons, double precision is preferred in scientific computing

- Many bits of a double are contaminated by error
  - Error from round-off, truncation, iteration, model, observation, …
  - Pushing error around and computing on it is wasteful

- To significantly reduce data movement, we must **make every bit count!**
  - Next generation floating types must be re-designed from ground up

POSITS [Gustafson 2017] are a new float representation that improves on IEEE



	IEEE 754 floating point	Posits: UNUM version 3.0
Bit Length	{16, 32, 64, 128}	fixed length but arbitrary
Sign	sign-magnitude (−0 ≠ +0)	two's complement (−0 = +0)
Exponent	fixed length (biased binary)	variable length (Golomb-Rice)
Fraction Map	linear ($\varphi(x) = 1 + x$)	linear ($\varphi(x) = 1 + x$)
Infinities	{−∞, +∞}	±∞ (single point at infinity)
NaNs	many (9 quadrillion)	one
Underflow	gradual (subnormals)	gradual (natural)
Overflow	1 / FLT_TRUE_MIN = ∞ (oops!)	never (exception: 1 / 0 = ±∞)
Base	{2, 10}	$2^{2^m} \in \{2, 4, 16, 256, \dots\}$

In terms of encoding scheme, IEEE and POSITS differ in one important way

- Both represent real value as $y = (-1)^s\, 2^e\, (1 + f)$
- **IEEE:** fixed-length **binary** encoding of exponent
- **POSITS:** variable-length **Golomb-Rice** encoding of exponent
  - Exponent, e, encoded as m trailing bits in binary ($e \bmod 2^m$), $1 + \lfloor e / 2^m \rfloor$ leading bits in unary
  - More fraction bits are available when exponent is small

IEEE float	IEEE double	POSIT(7)
$e = D(1\ x) = 1 + x$ 1-bit exponent "sign" 7-bit exponent magnitude x	$e = D(1\ 000\ x) = 1 + x$	$e = D(1\ 0\ x) = x$
	$e = D(1\ 001\ x) = 129 + x$	$e = D(1\ 10\ x) = 128 + x$
	$e = D(1\ 010\ x) = 257 + x$	$e = D(1\ 110\ x) = 256 + x$
	…	…
	$e = D(1\ 111\ x) = 897 + x$	$e = D(1\ 11111110\ x) = 896 + x$

Related work: Universal coding of positive integers [Elias 1975]

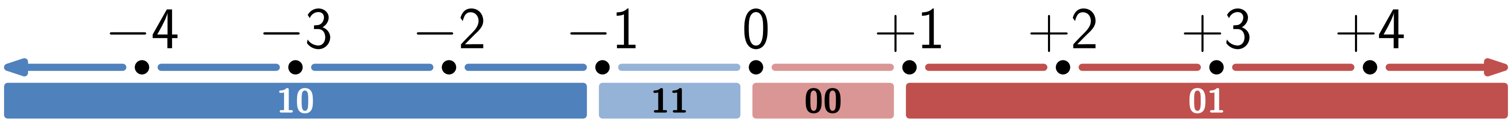
- Decompose integer $z \geq 1$ as $z = 2^e + r$
  - $e \geq 0$ is **exponent**
  - $r = z \bmod 2^e$ is e-bit **residual**

- Elias proposed three "prefix-free" variable-length codes for integers
  - Elias γ code is equivalent to POSIT(0) [Gustafson & Yonemoto 2017]
  - Elias δ code is equivalent to URR [Hamada 1983]

	Elias γ code	Elias δ code	Elias ω code
Exponent	unary	γ	ω (recursive)
Code(1)	0	0	0
Code($2^e + r$)	1^e 0 r	1 $\gamma(e)$ r	1 $\omega(e)$ r
Code($17 = 2^4 + 1$)	1111 0 0001	1 11 0 00 0001	1 1 1 0 0 00 0001

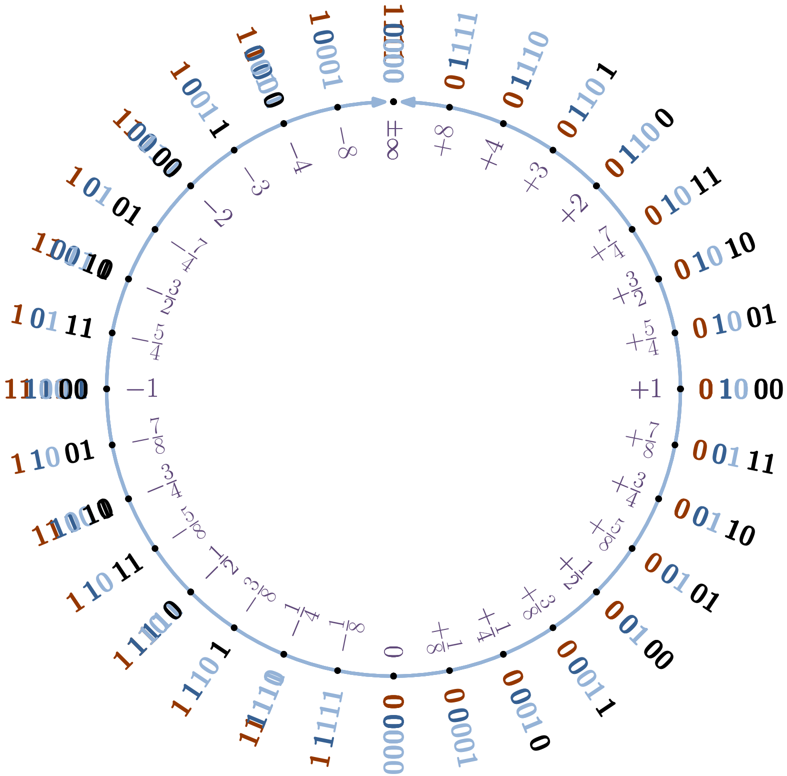
We extend Elias codes from positive integers to reals

- From $z \in \mathbb{N}$ (positive integers) to $y \in \mathbb{R}$ (reals)
  - **Rationals**: $1 \le z < y < z + 1$ encoded by appending fraction bits (as in IEEE, POSITS)
  - **Subunitaries**: $0 < y < 1$ encoded via two's complement exponent (as in POSITS)
  - **Negatives**: $y < 0$ encoded via two's complement binary representation (as in POSITS)
  - 2-bit prefix tells where we are on the real line (as in POSITS)



POSITS, Elias recursively refine intervals (0, ±1), (±1, ±∞)
Example: base-2 posits (aka. Elias γ)

- sign bit
- exponent sign
- exponent value
- fraction value



Beyond POSITS and Elias: NUMREP templated framework

- NUMREP is a modular C++ framework for defining number systems
  - **Exponent coding scheme** (unary, binary, Golomb-Rice, gamma, omega, …)
  - **Fraction map** (linear, reciprocal, exponential, rational, quadratic, logarithmic, …)
    - *Conjugate* fraction maps for sub- & superunitaries enable reciprocal closure
  - Handling of **under- & overflow**
  - **Rounding** rules (to nearest, toward $\{-\infty, 0, +\infty\}$)

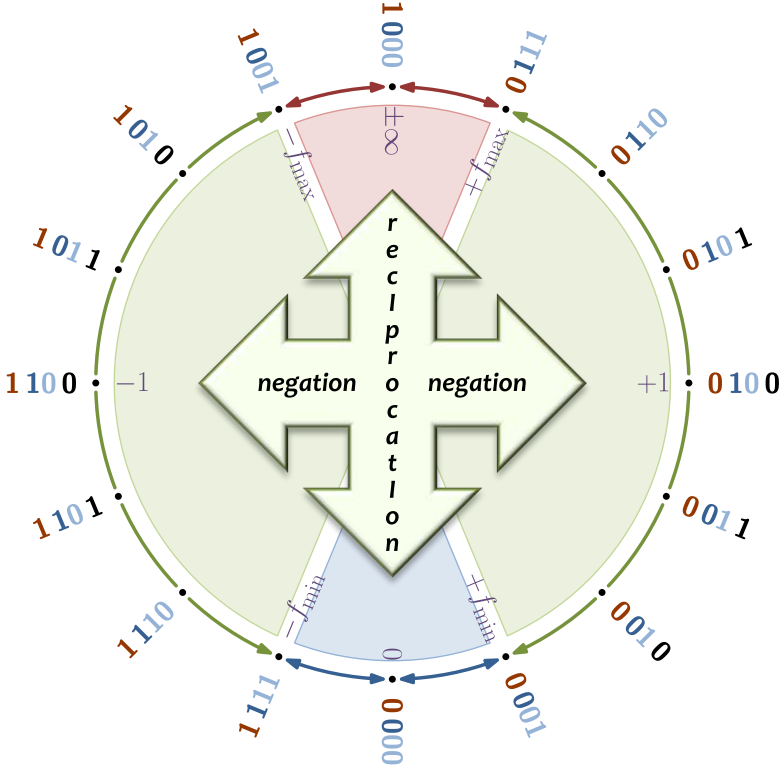
- NUMREP unifies IEEE, POSITS, Elias, URR, LNS, … , under a single schema
  - Uses auxiliary **arithmetic type** to perform numerical computations (e.g. IEEE, MPFR)
  - Uses **operator overloading** to mimic intrinsic floating types
  - Supports 8, 16, 32, 64-bit types

Lindstrom et al., "Universal coding of the reals: Alternatives to IEEE floating point," *Conference for Next Generation Arithmetic*, 2018

NUMREP is a powerful but complex framework—let's take a simplified view

Many useful NUMREPS are given by simple interpolation and extrapolation rules (plus closure under negation)

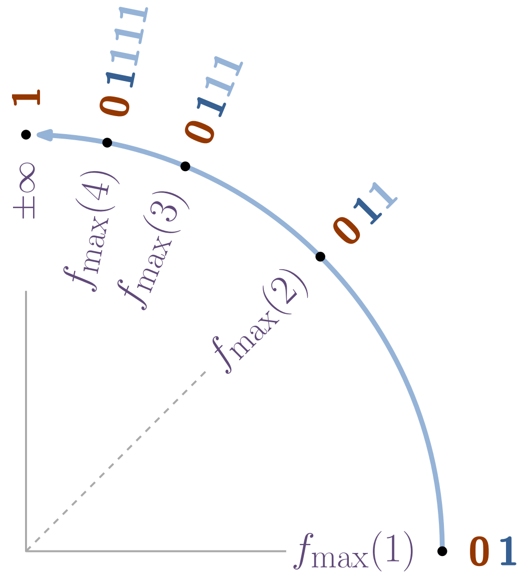
- extrapolation on $(f_{\max}, \infty)$
- interpolation on $(f_{\min}, f_{\max})$
- reciprocation on $(0, f_{\min})$



Extrapolation gives next $f_{\max}$ between previous $f_{\max}$ and $\pm\infty$ when adding one more bit of precision

- **Extrapolation rule:** $1 \le f_{\max}(p) < f_{\max}(p+1) < \infty$

type	$f_{\max}(p+1)$	sequence
Unary	$1 + f_{\max}(p)$	1, 2, 3, 4, 5, …
Elias γ	$2 \times f_{\max}(p)$	1, 2, 4, 8, 16, …
POSITS (base b)	$b \times f_{\max}(p)$	1, b, b^2, b^3, b^4, …
Elias δ	$f_{\max}(p)^2$	1, 2, 4, 16, 256, …
Elias ω	$2^{f_{\max}(p)}$	1, 2, 4, 16, 65536, …



- **Reciprocation rule:** $f_{\min}(p) = 1 / f_{\max}(p)$

Interpolation rule generates new number g(*a*, *b*) between two finite positive numbers *a* < *b*

- For POSITS, Elias {γ, δ, ω}:

$$g(a,b) = \begin{cases} \dfrac{a+b}{2} & \text{if } b \le 2a \\ 2^{g(\lg a,\, \lg b)} & \text{otherwise} \end{cases}$$

- Examples
  - $g(2, 4) = 3$ — arithmetic mean
  - $g(4, 16) = 2^{g(2,4)} = 2^3 = 8$ — geometric mean
  - $g(16, 65536) = 2^{g(4,16)} = 2^{2^{g(2,4)}} = 2^{2^3} = 2^8 = 256$ — "hypergeometric" mean (for ω only)

- For LNS:

$$g(a,b) = \sqrt{ab}$$

FLEX (FLexible EXponent): NUMREP on a shoestring

- Templated on ***generator*** that implements two rules
  - Interpolation function, $g(a, b)$
  - Extrapolation recurrence, $a_{i+1} = f(a_i) = g(a_i, \infty)$

- Rules + bisection implement encoding, decoding, rounding, fraction map
  - Recursively bisect $(-\infty, +\infty)$ using applicable interpolation or extrapolation rule
    - $g(-\infty, +\infty) = 0$
    - $g(0, \pm\infty) = \pm 1$
  - Exploit symmetry of negation, reciprocation
  - **Encode:** bracket number and recursively test if less (0) or greater (1) than bisection point
  - **Decode:** narrow interval toward lower (0) or upper (1) bound; return final lower bound
  - **Round:** round number to lower bound if less than bisection point, otherwise to upper
  - **Map:** given by interpolation rule

- NOTE: Not very performant, but great for experimentation & validation

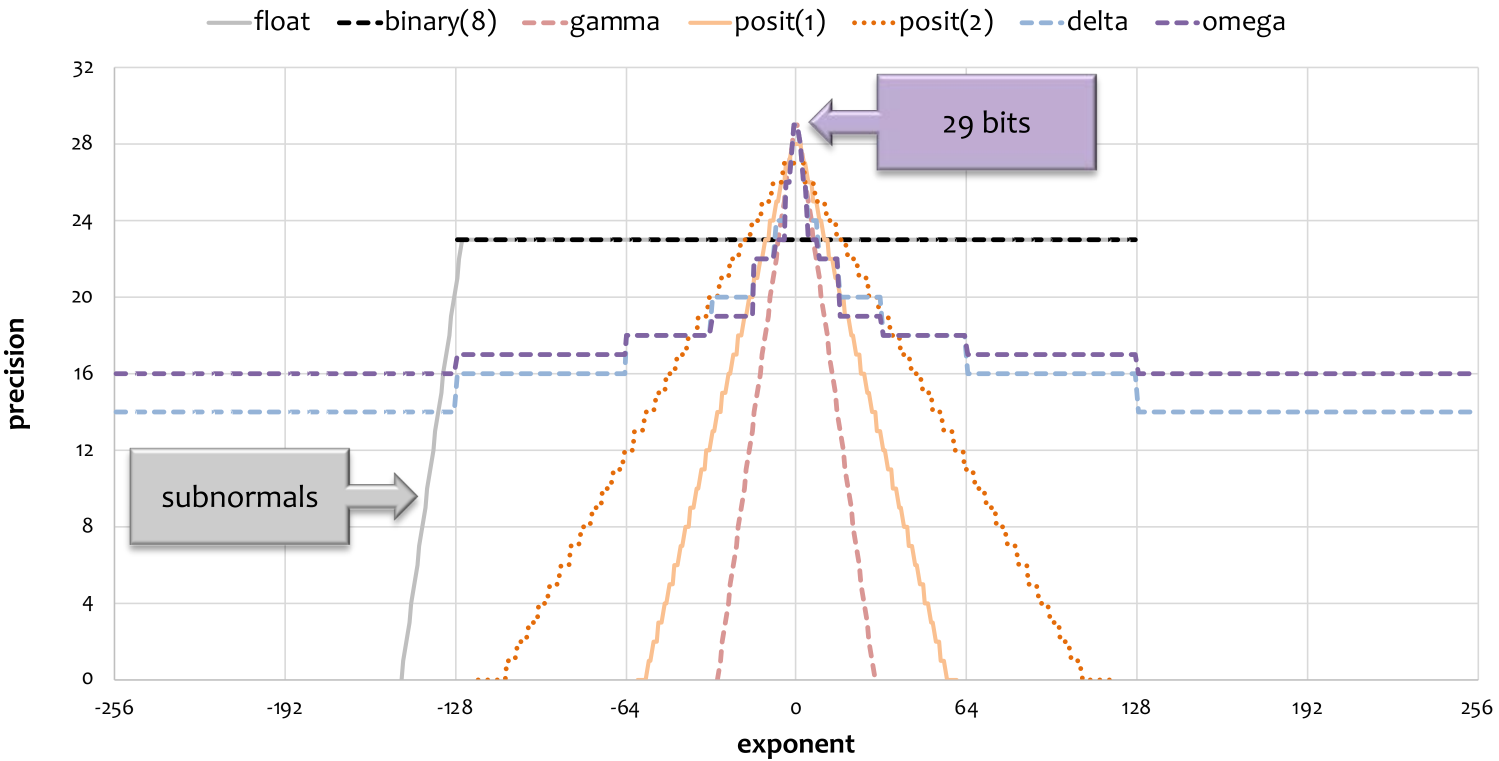
FLEX's POSIT implementation is 8 lines of code

```
// posit generator with m-bit exponent and base 2^(2^m)
template <int m = 0, typename real = flex_real>
class Posit {
public:
    real operator()(real x) const { return real(base) * x; }
    real operator()(real x, real y) const { return real(2) * x >= y ? (x + y) / real(2) : std::sqrt(x * y); }
protected:
    static const int base = 1 << (1 << m);
};
```

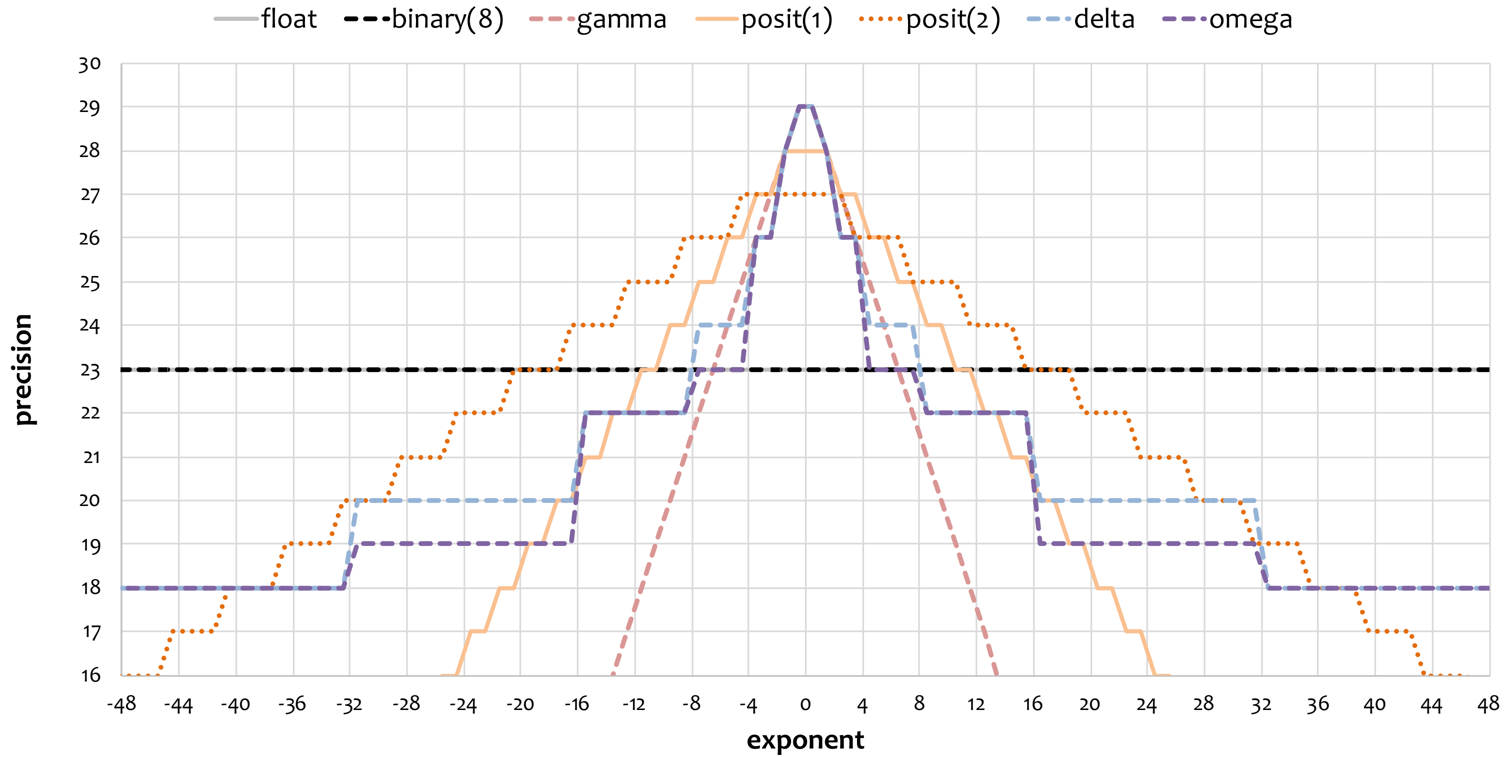
Elias delta and the Kessel Run: What is the distance to Proxima Centauri?

Quantity	Format	Sign	Exponent	Fraction	Error
1.3 parsecs	IEEE	0	01111111	01001100111101100101011	error = 1.2e−08
	ELIAS δ	0	$\underbrace{10}_{\text{2 bits}}$	01001100111101100101010**111000**	error = 4.8e−10
4.2 lightyears	IEEE	0	10000001	00001111011111101001000	error = 5.6e−08
	ELIAS δ	0	$\underbrace{11100}_{\text{5 bits}}$	00001111011111101001000**100**	error = 9.0e−11
4.0×10^{16} meters	IEEE	0	10110110	000111010010101000**10101**	error = 1.5e−08
	ELIAS δ	0	$\underbrace{1111111010111}_{\text{13 bits}}$	000111010010101001	error = 1.2e−06
2.4×10^{51} Planck lengths	IEEE	0	11111111	00000000000000000000000	error = ∞
	ELIAS δ	0	$\underbrace{11111111100101010}_{\text{17 bits}}$	**10101000110001**	error = 1.4e−05

Variable-length exponents lead to tapered precision: 6-9 more bits of precision than IEEE for numbers near one



Tapered precision (close-up): tension between precision and dynamic range

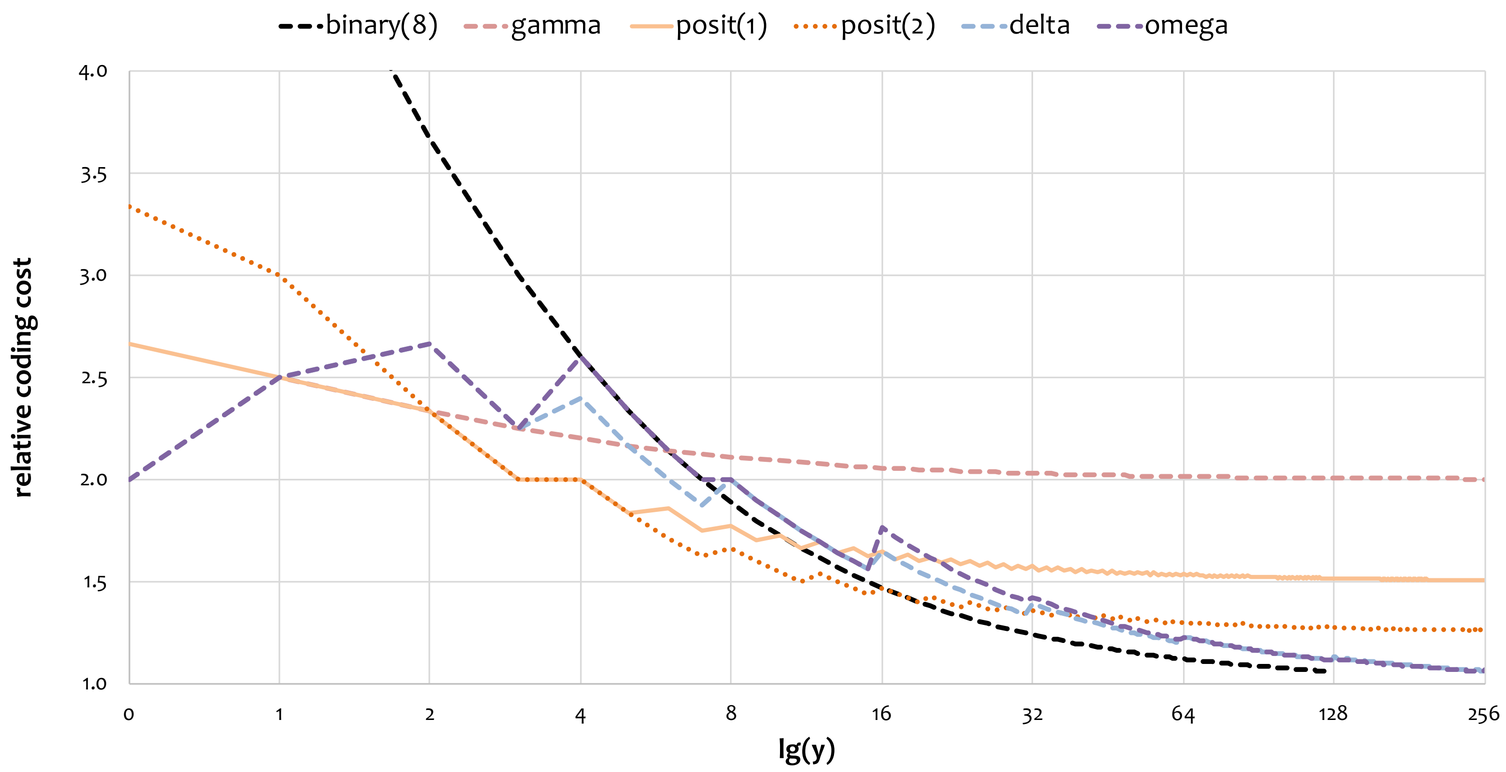


Elias delta and omega are asymptotically optimal universal representations

- Universality property (POSITS, Elias {γ, δ, ω}, but not IEEE)
  1. Each integer is represented by a ***prefix code***
     - No codeword is a prefix of any other codeword
     - Codeword length is self-describing—remaining available bits represent fraction
  2. Integer representation has ***monotonic length***
     - Larger integers have longer codewords
  3. Codeword length of integer *y* is $\boldsymbol{O(\lg y)}$
     - Codeword length is proportional to the number of significant bits

- Asymptotic optimality property (Elias {δ, ω})
  - Relative cost of coding exponent (leading-one position) vanishes in the limit

Elias delta and omega are asymptotically optimal: exponent overhead approaches zero in the limit



Fraction maps dictate how fraction bits map to values

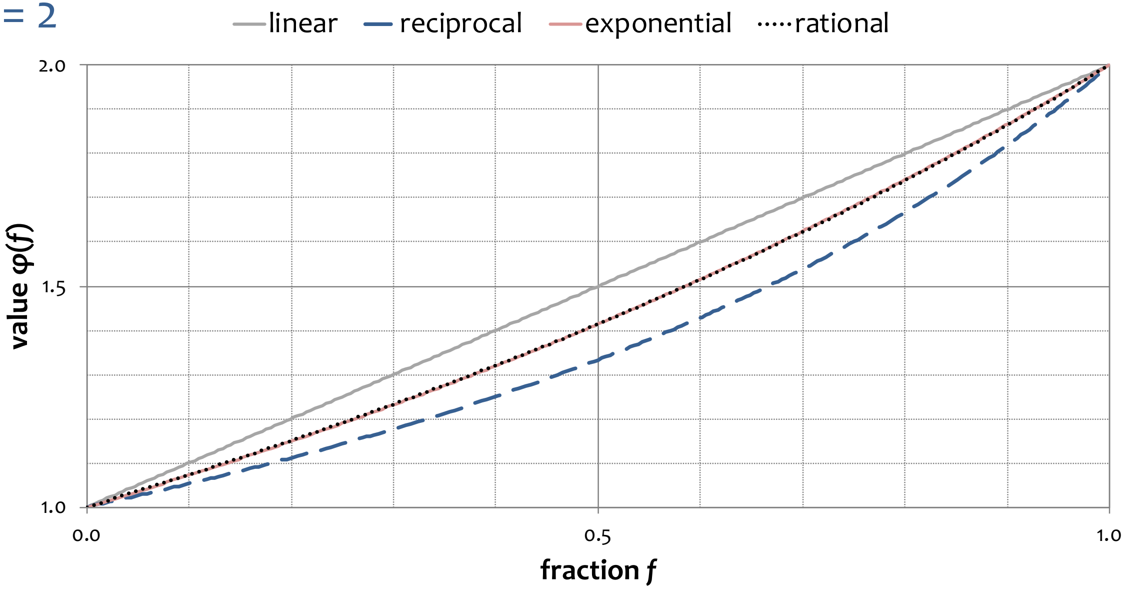
- So far we have assumed that fraction (significand), $f \in [0, 1)$, is mapped linearly
  - $y = (-1)^s\, 2^e\, (1 + f)$
  - We may replace $(1 + f)$ with transfer function $\varphi(f)$

- Fraction map, $\varphi : [0, 1) \longrightarrow [1, 2)$, maps fraction bits, f, to value, $\varphi(f)$
  - Subunitary map φ^-: $|y| < 1$
  - Superunitary map φ^+: $|y| \geq 1$

map	φ(f)	notes
Linear	$1 + f$	*introduces implicit leading-one bit*
Linear reciprocal	$2 / (2 - f)$	*conjugate with linear map ⇒ reciprocal closure*
Exponential	2^f	LNS *(logarithmic number system):* $y = 2^e\, 2^f = 2^{e+f}$
Linear rational	$(1 + p\, f) / (1 - q\, f)$	$p = \sqrt{2} - 1$, $q = (1 - p) / 2$

Conjugate pair (φ^-, φ^+) guarantees reciprocal closure

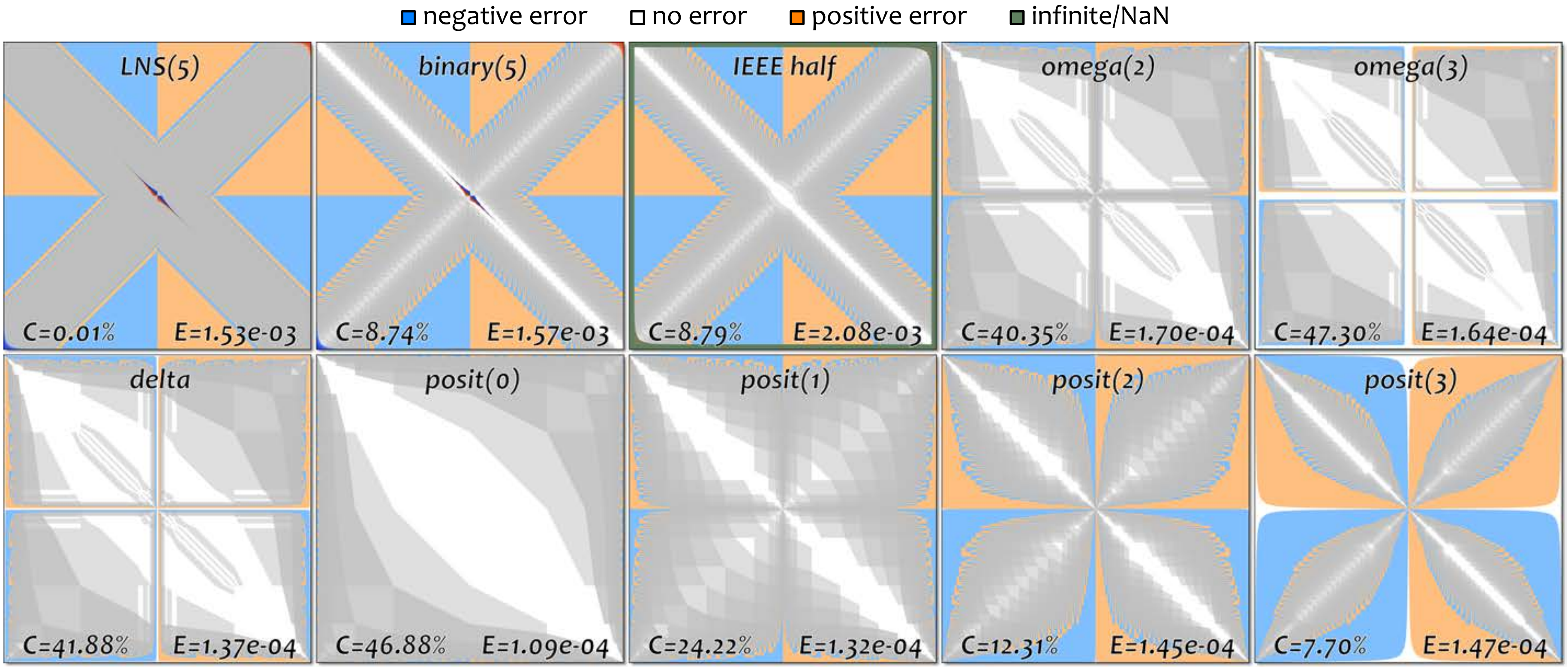
- Conjugacy: $\varphi^-(f)\ \varphi^+(1 - f) = 2 \quad 0 \le f \le 1$
  - E.g. $2 / (2 - f) \times (1 + (1 - f)) = 2$
- C^n continuity: $\varphi^{(n)}(1) / \varphi^{(n)}(0) = 2$



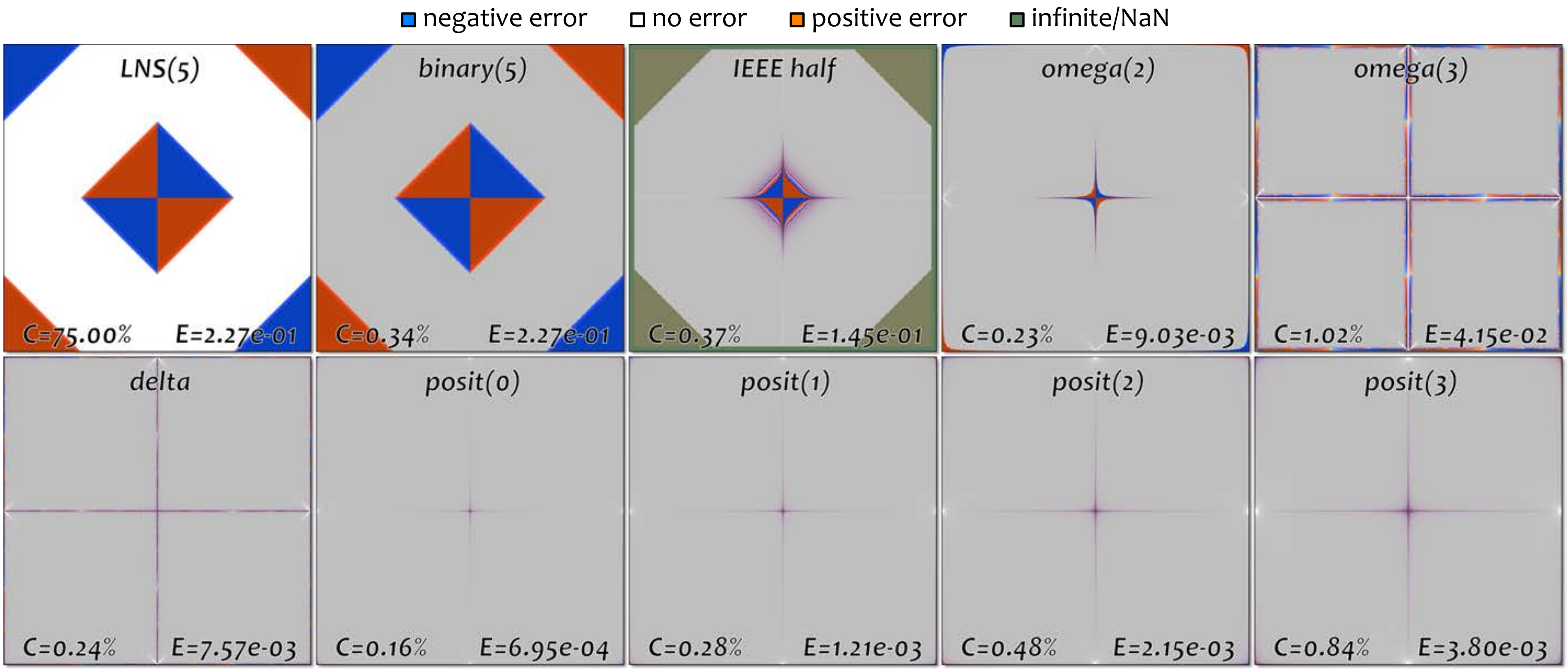
We present extensive results that span a spectrum of simple to increasingly complex numerical computations

- **Arithmetic closure** and relative error (vs. analytic solution) $z = x + y$
  - Addition and multiplication of 16-bit operands
- **Addition** of long floating-point sequences (vs. analytic solution) $s = \sum_i a_i$
  - Using naïve and best-of-breed addition algorithms
- **Matrix inversion** (vs. analytic solution) $A = H^{-1}$
  - LU-based inversion of Hilbert and Vandermonde matrices
- Symmetric matrix **eigenvalues** (vs. analytic solution) $\Lambda = QAQ^T$
  - QR-based dense eigenvalue solver
- Euler2D **PDE solver** (vs. IEEE quad precision) $\partial_t u + \nabla \cdot f(u) = 0$
  - Complex physics involving interacting shock waves

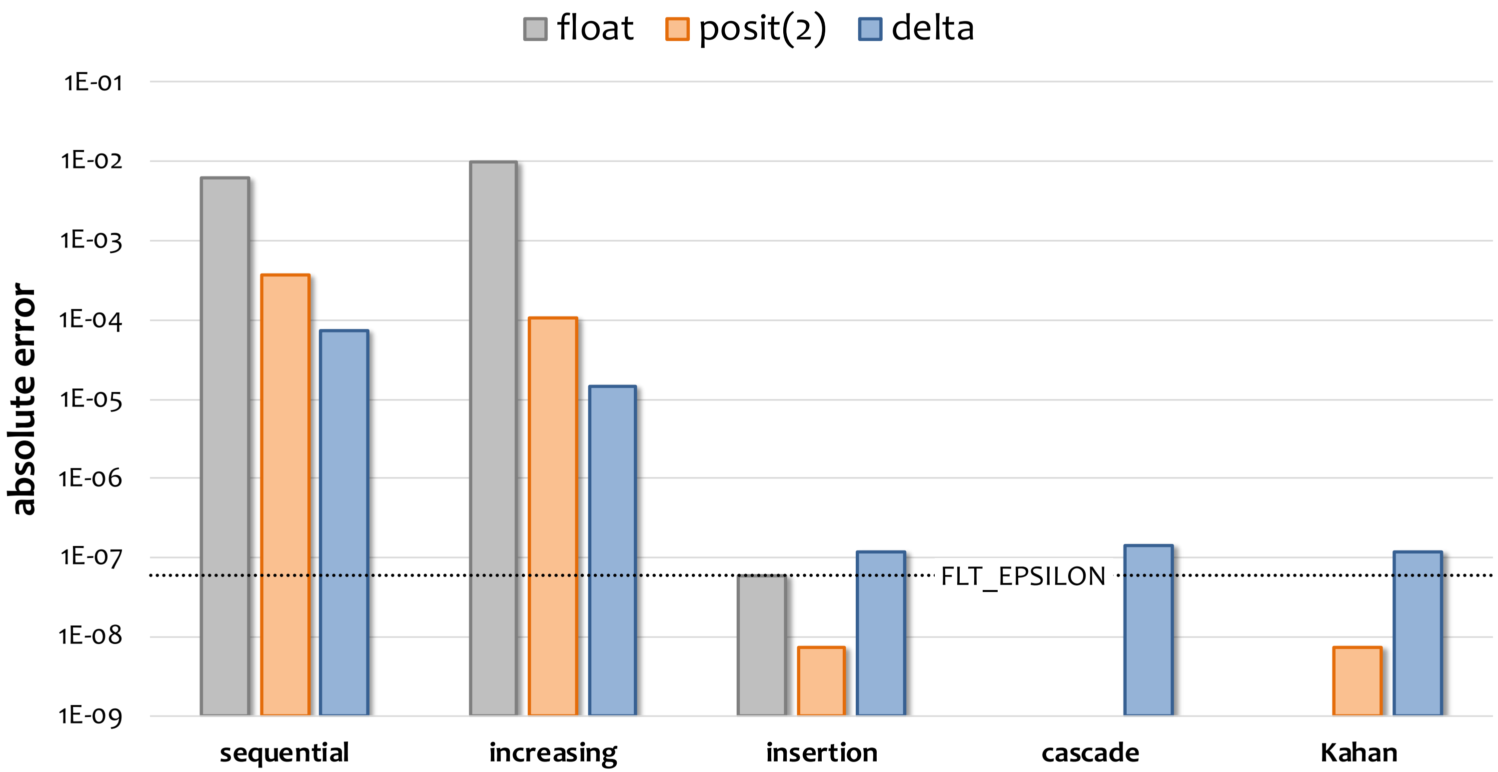
Closure rate (C) and mean relative error (E) for 16-bit addition suggest POSIT(0) (aka. Elias gamma) performs best



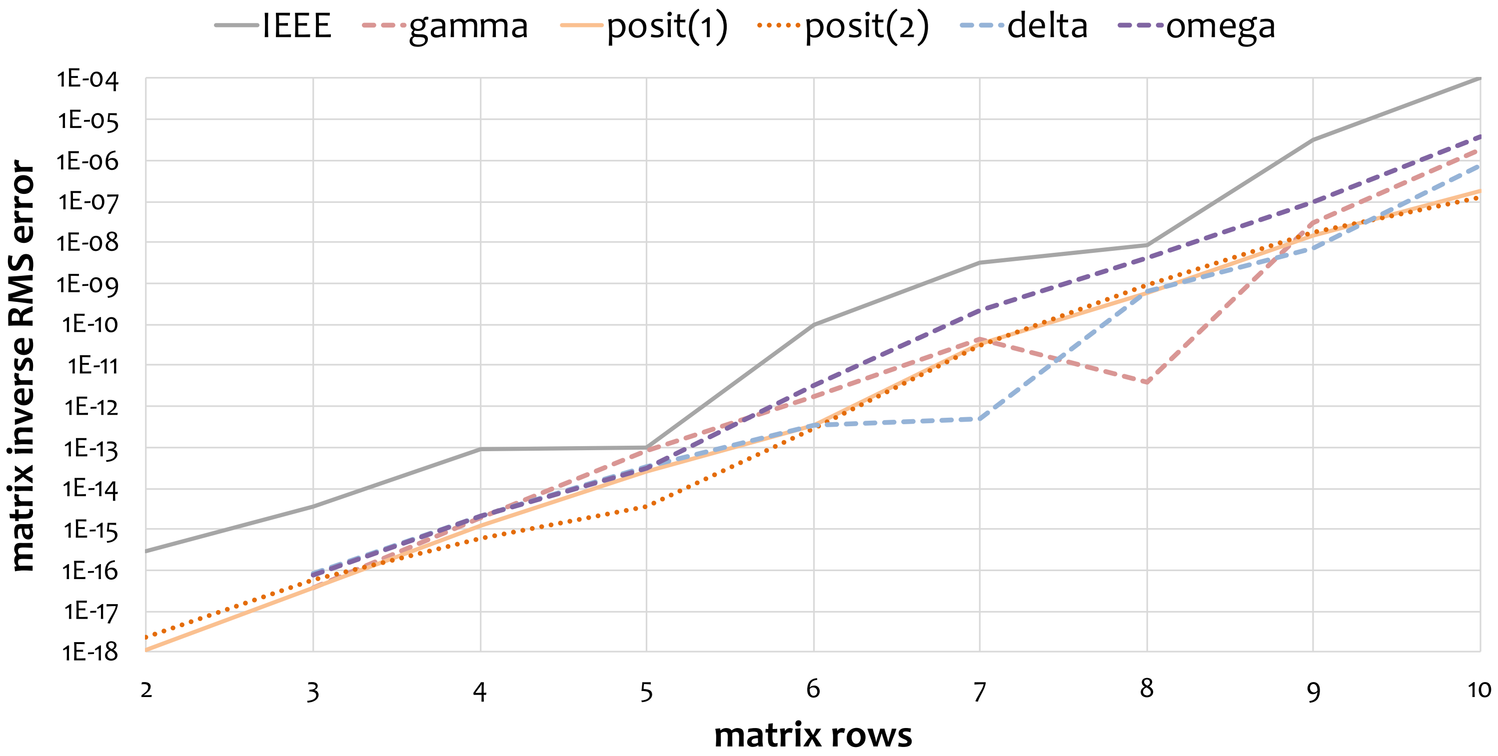
Optimal multiplicative closure of LNS does not imply superior relative errors



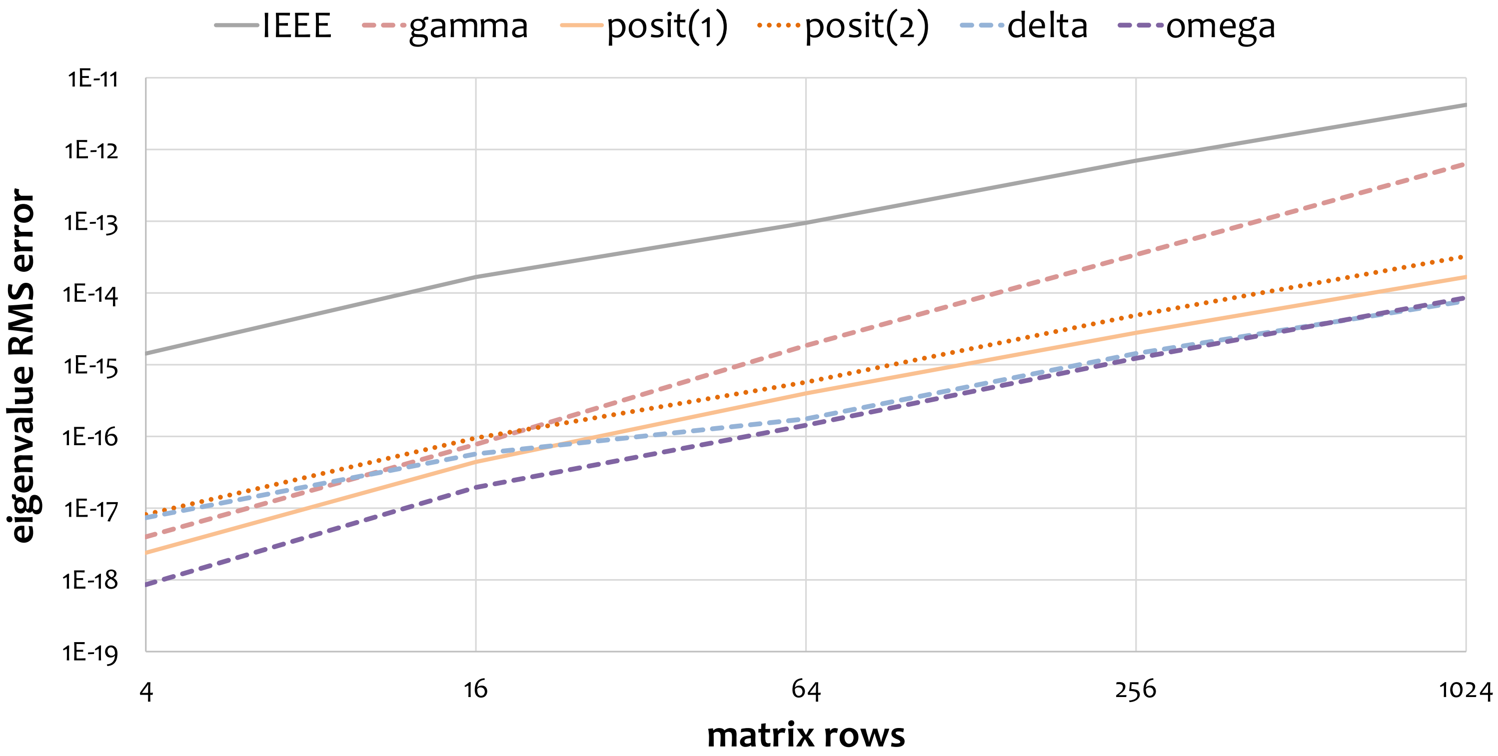
Simple summation algorithms benefit from tapered precision: Sum of Gaussian PDF and its first derivative



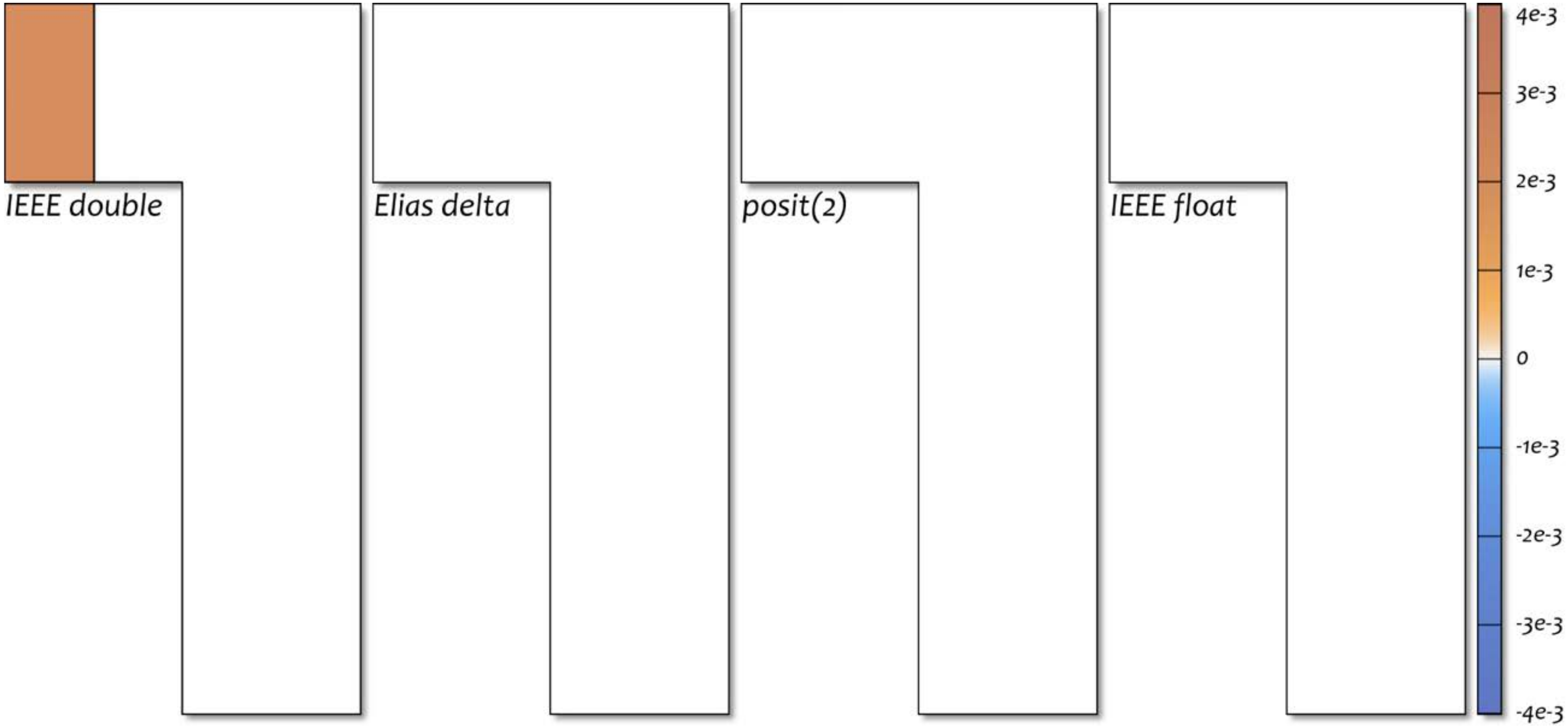
New types excel in 64-bit Hilbert matrix inversion (Eigen3)



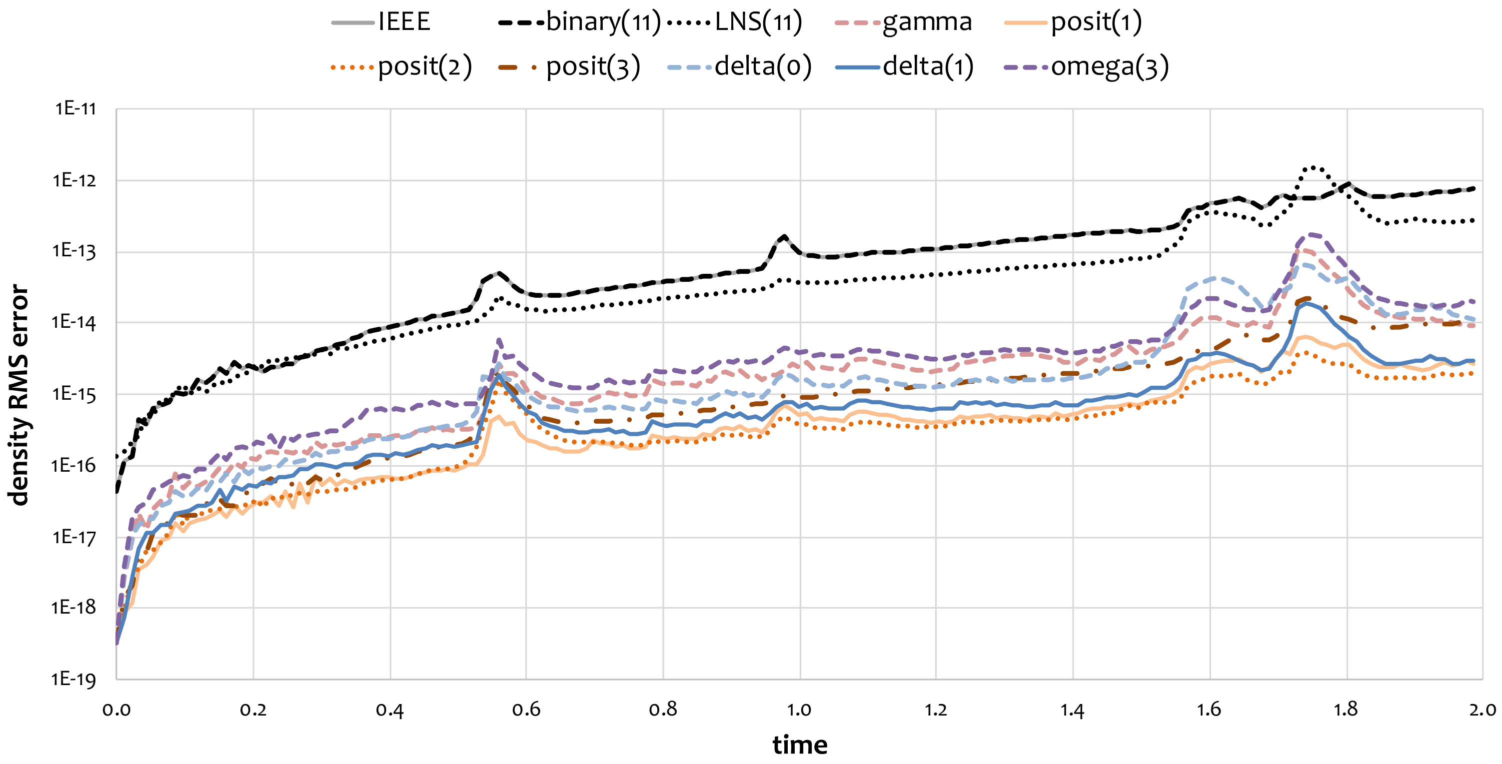
Elias outperforms IEEE by O(10^3) in 64-bit eigenvalue accuracy



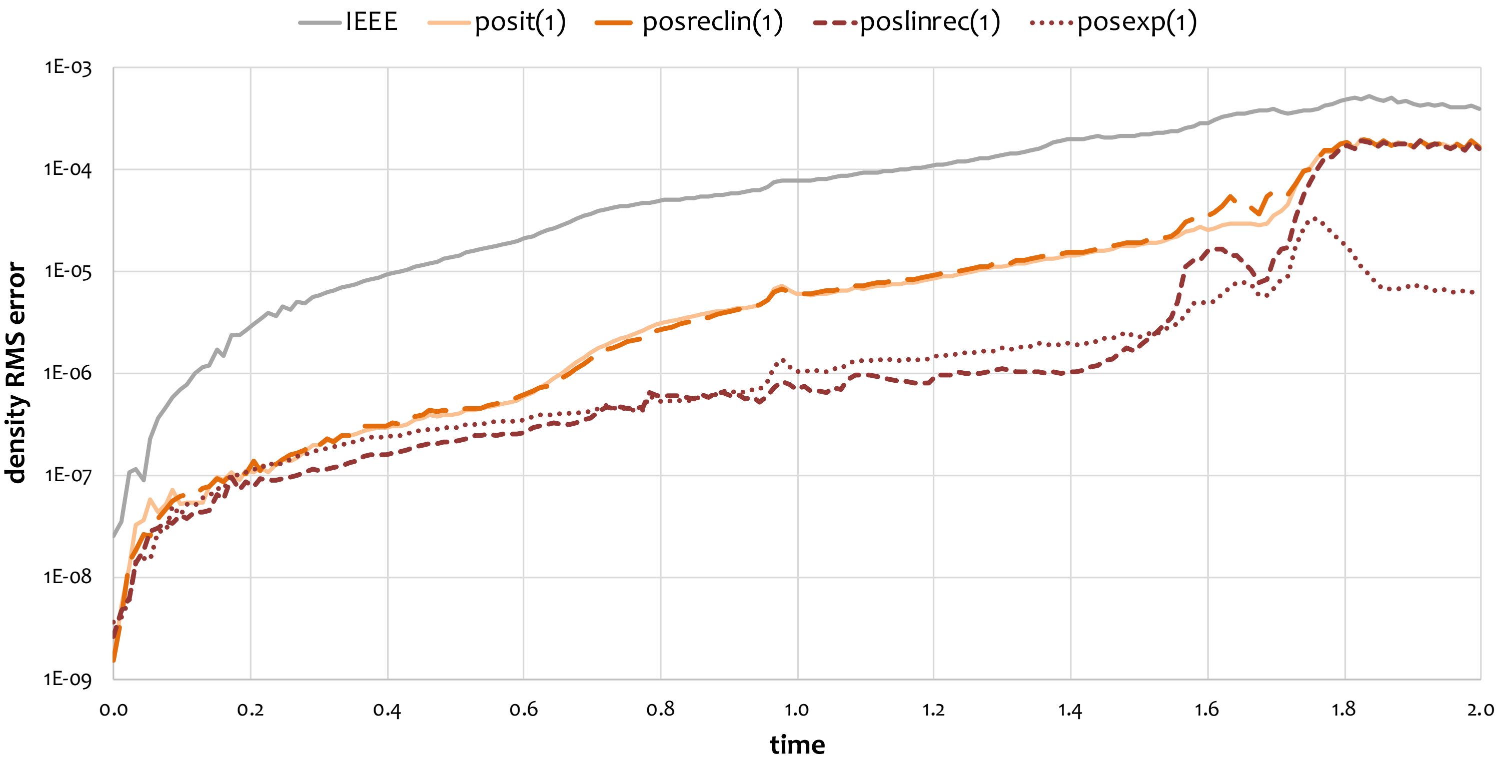
Euler2D shock propagation illustrates benefits of new types



IEEE consistently is the least accurate floating-point representation in numerical calculations (64-bit types)

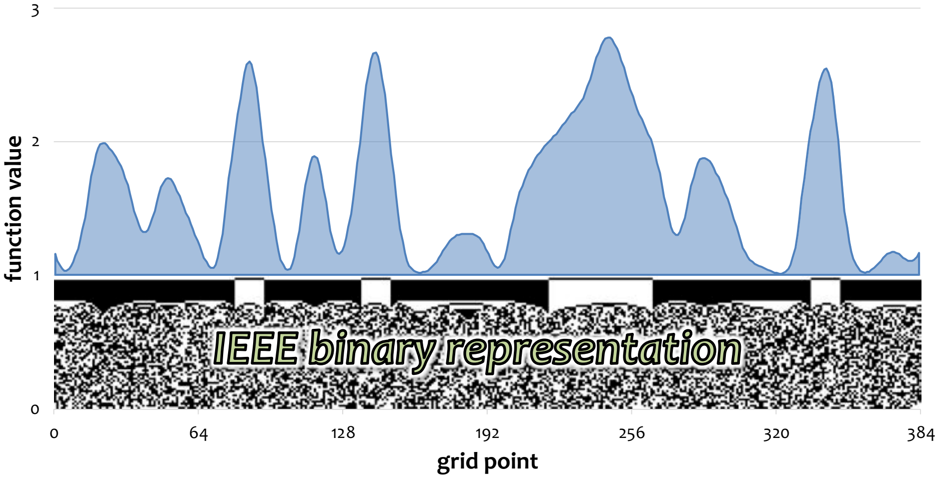


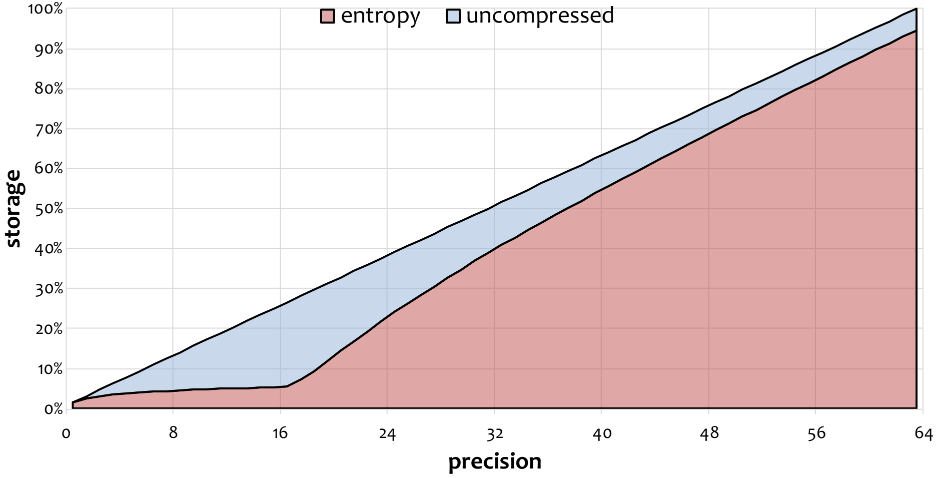
Nonlinear fraction maps sometimes improve accuracy substantially (32-bit types)



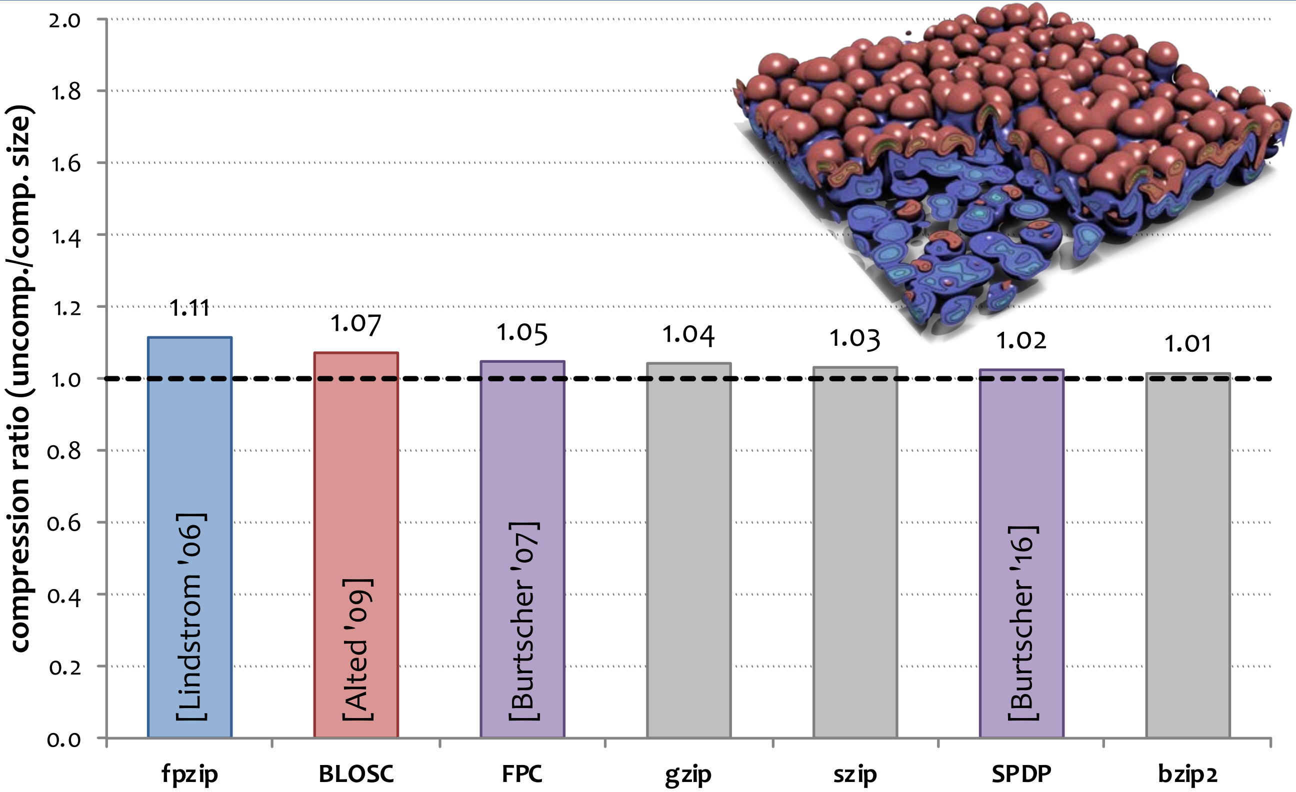
Beyond IEEE and posit representations of $\mathbb{R}$: Compressed representations of $\mathbb{R}^n$

- Many numerical computations involve continuous fields
  - E.g. partial differential equations over $\mathbb{R}^2$, $\mathbb{R}^3$
  - Nearby scalars on Cartesian grids have similar values
    - In statistical speak, fields exhibit ***autocorrelation***
    - Such redundancy is not exploited by any of the representations discussed so far



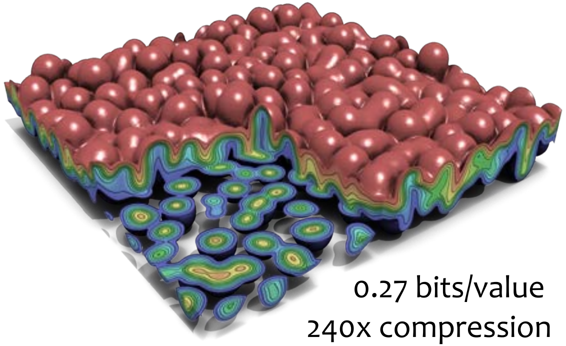


(64-bit) floating-point data does not compress well losslessly



Lossy compression enables greater reduction, but is often met with skepticism by scientists

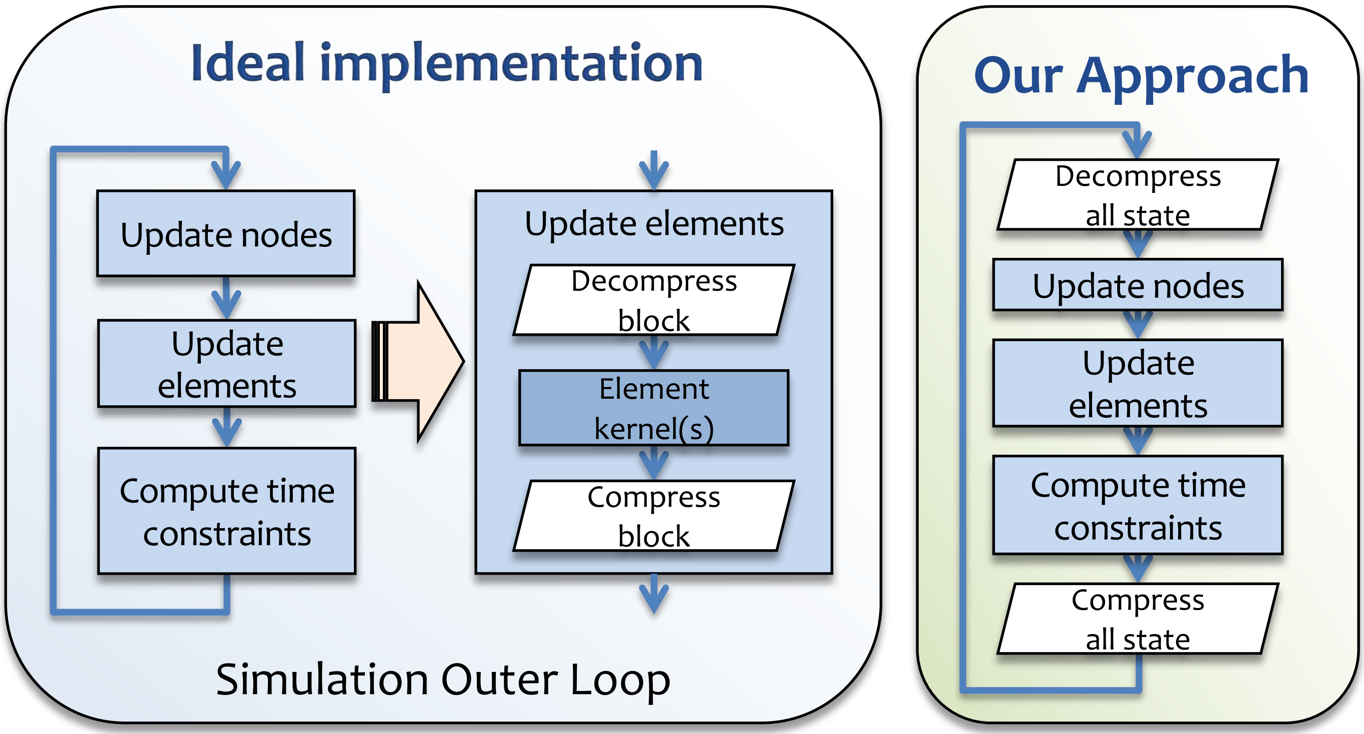
- Large improvements in compression are possible by allowing even small errors
  - Simulation often computes on meaningless bits
    - Round-off, truncation, iteration, model **errors abound**
    - Last few floating-point bits are effectively **random noise**



0.27 bits/value
240x compression

- Still, lossy compression often makes scientists nervous
  - Even though lossy **data reduction** is ubiquitous
    - **Decimation** in space and/or time (e.g. store every 100 time steps)
    - **Averaging** (hourly vs. daily vs. monthly averages)
    - **Truncation** to single precision (e.g. for history files)
  - State-of-the-art compressors support **error tolerances**

Can lossy-compressed in-memory storage of numerical simulation state be tolerated?



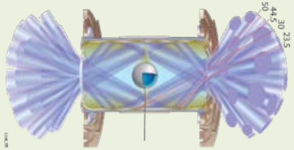
Using lossy FPZIP to store simulation state compressed, we have shown that 4x lossy compression can be tolerated

Lagrangian shock hydrodynamics

- QoI: *radial shock position*
- 25 state variables compressed over 2,100 time steps
- At **4x compression**, relative **error < 0.06%**

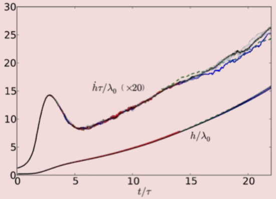
Laser-plasma multi-physics

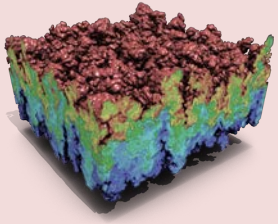
- QoI: *backscattered laser energy*
- At **4x compression**, relative **error < 0.1%**



High-order Eulerian hydrodynamics

- QoI: *Rayleigh-Taylor mixing layer thickness*
- 10,000 time steps
- At **4x compression**, relative **error < 0.2%**

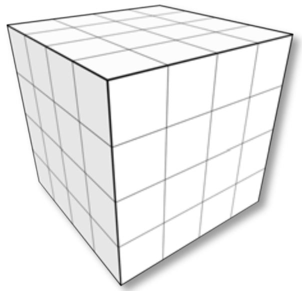




Lossy compression of state is viable, but streaming compression *increases* data movement—need inline compression

ZFP is an inline compressor for floating-point arrays

- Inspired by ideas from h/w texture compression
  - *d*-dimensional array divided into blocks of 4^d values
  - Each block is independently (de)compressed
    - e.g. to a user-specified number of bits or quality
  - Fixed-size blocks $\Rightarrow$ **random read/write access**
  - (De)compression is done **inline**, on demand
  - **Write-back cache** of uncompressed blocks limits data loss



- Compressed arrays via C++ operator overloading
  - Can be dropped into existing code by changing type declarations
  - double a[n] $\Leftrightarrow$ std::vector<double> a(n) $\Leftrightarrow$ zfp::array<double> a(n, **precision**)

Lindstrom, "Fixed-rate compressed floating-point arrays," *IEEE Transactions on Visualization and Computer Graphics*, 2014

ZFP's C++ compressed arrays can replace STL vectors and C arrays with minimal code changes

// example using STL vectors

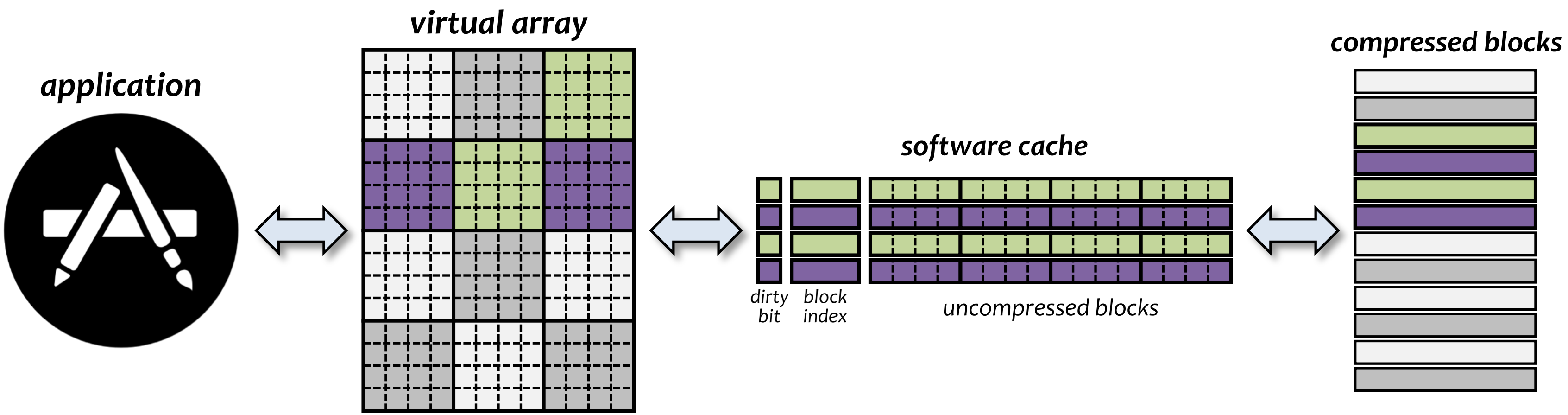
```
std::vector<double> u(nx * ny, 0.0);
u[x0 + nx*y0] = 1;
for (double t = 0; t < tfinal; t += dt) {
    std::vector<double> du(nx * ny, 0.0);
    for (int y = 1; y < ny - 1; y++)
        for (int x = 1; x < nx - 1; x++) {
            double uxx = (u[(x-1)+nx*y] - 2*u[x+nx*y] + u[(x+1)+nx*y]) / dxx;
            double uyy = (u[x+nx*(y-1)] - 2*u[x+nx*y] + u[x+nx*(y+1)]) / dyy;
            du[x + nx*y] = k * dt * (uxx + uyy);
        }
    for (int i = 0; i < u.size(); i++)
        u[i] += du[i];
}
```

// example using ZFP arrays

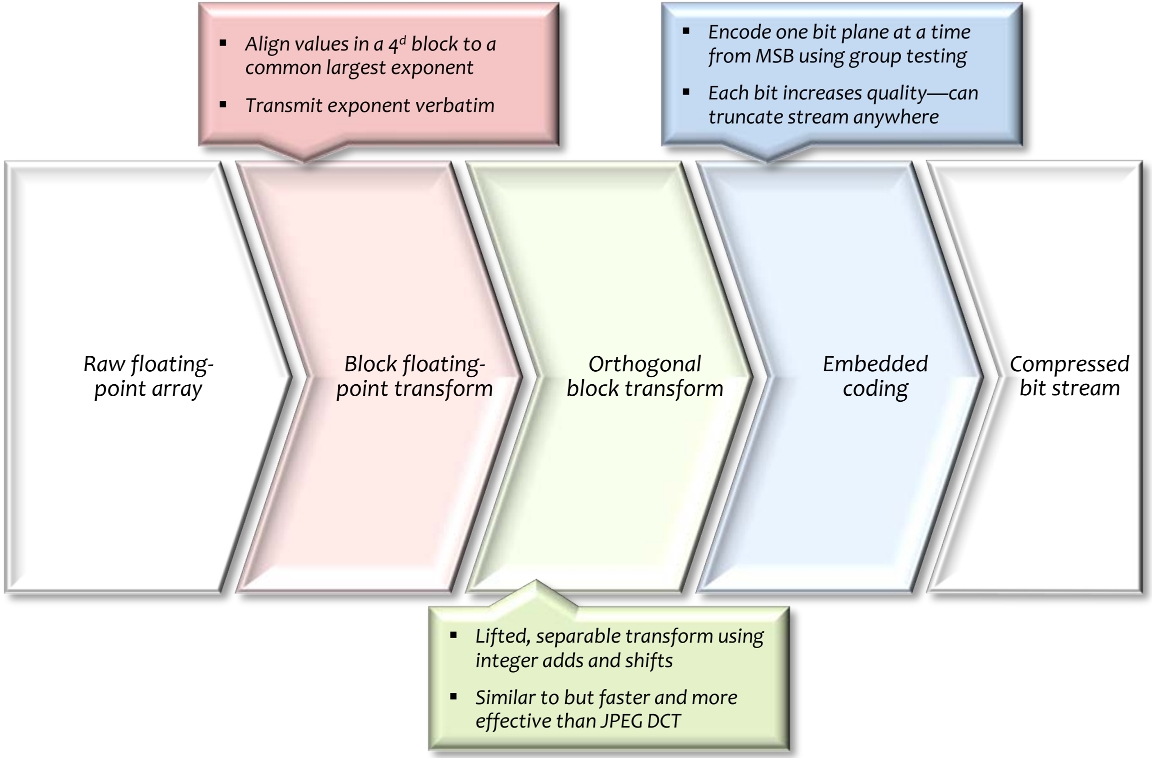
```
zfp::array2<double> u(nx, ny, bits_per_value);
u(x0, y0) = 1;
for (double t = 0; t < tfinal; t += dt) {
    zfp::array2<double> du(nx, ny, bits_per_value);
    for (int y = 1; y < ny - 1; y++)
        for (int x = 1; x < nx - 1; x++) {
            double uxx = (u(x-1, y) - 2*u(x, y) + u(x+1, y)) / dxx;
            double uyy = (u(x, y-1) - 2*u(x, y) + u(x, y+1)) / dyy;
            du(x, y) = k * dt * (uxx + uyy);
        }
    for (int i = 0; i < u.size(); i++)
        u[i] += du[i];
}
```

- required changes
- optional changes for improved readability

ZFP arrays limit data loss via a small write-back cache

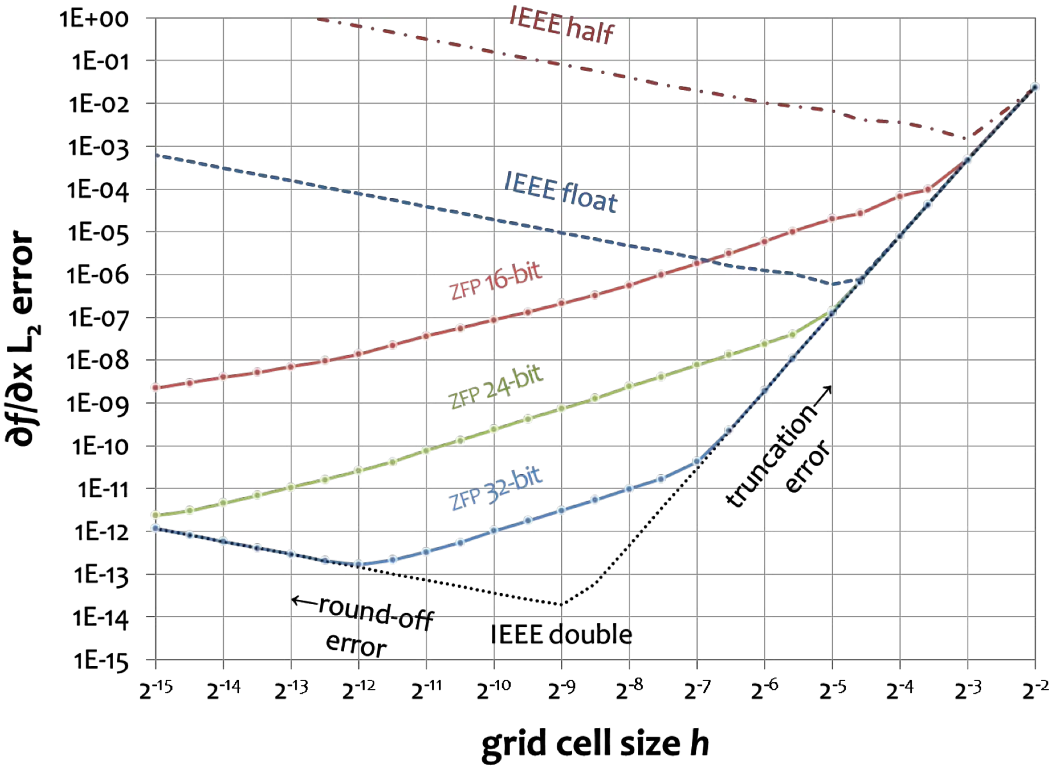


The ZFP compressor is comprised of three distinct components



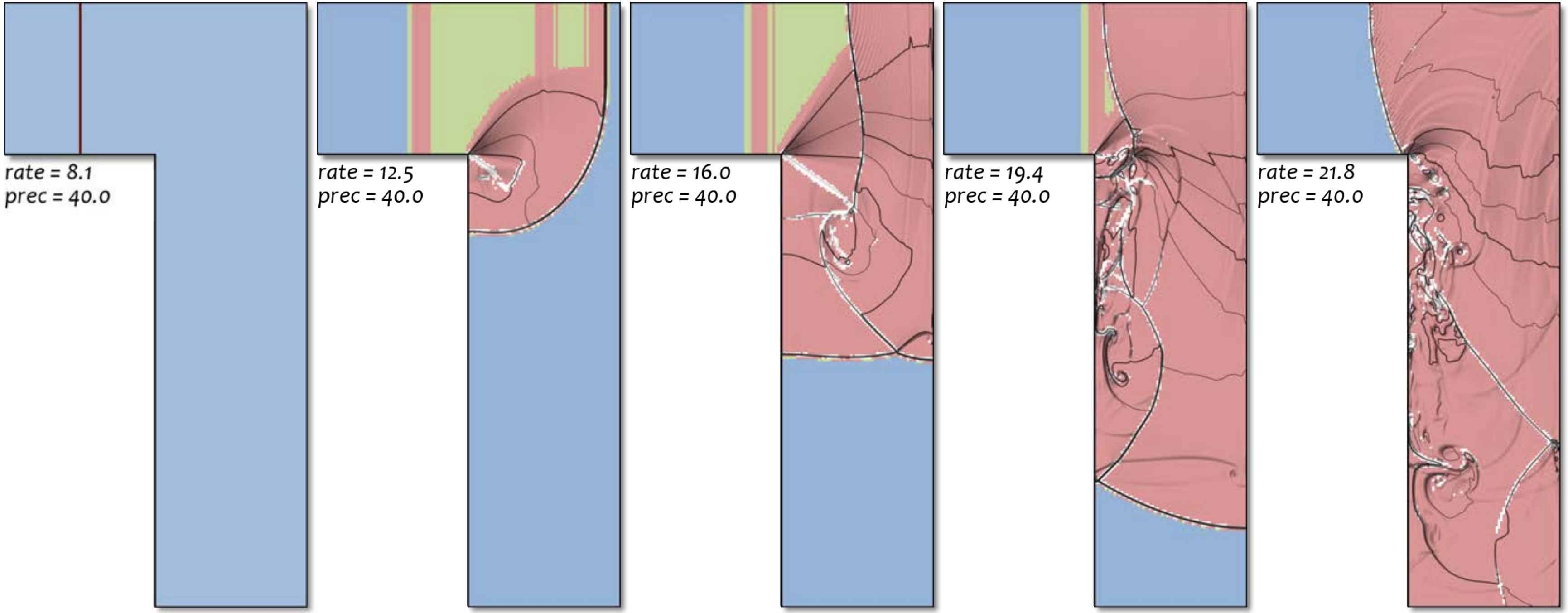
6-bit ZFP gives one more digit of accuracy than 32-bit IEEE in 2nd, 3rd derivative computations (Laplacian and highlight lines)

ZFP *improves* accuracy in finite difference computations using less precision than IEEE

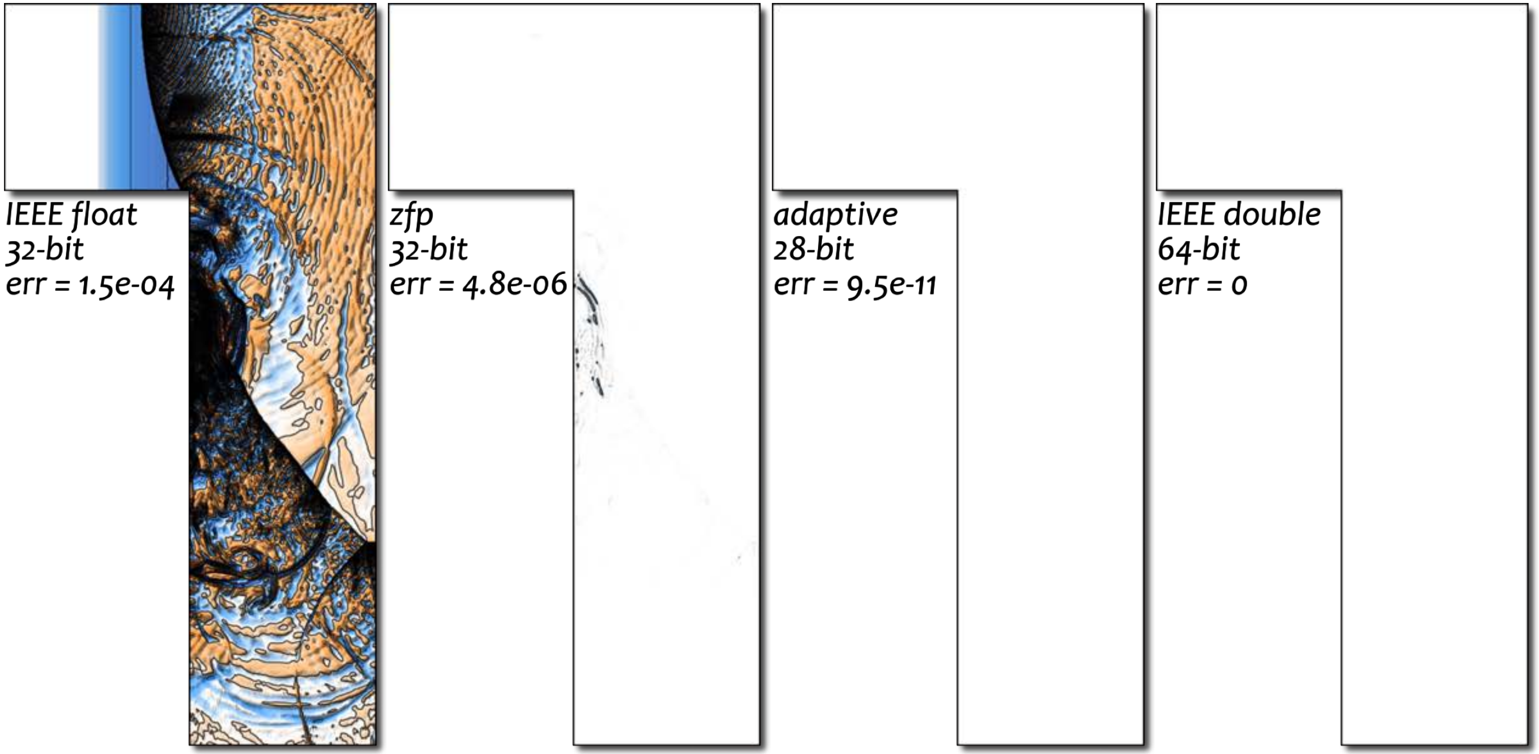


ZFP variable-rate arrays adapt storage spatially and allocate bits to regions where they are most needed

8 bits/value *16 bits/value* *32 bits/value* *64 bits/value*



ZFP adaptive arrays improve accuracy in PDE solution over IEEE by 6 orders of magnitude using less storage



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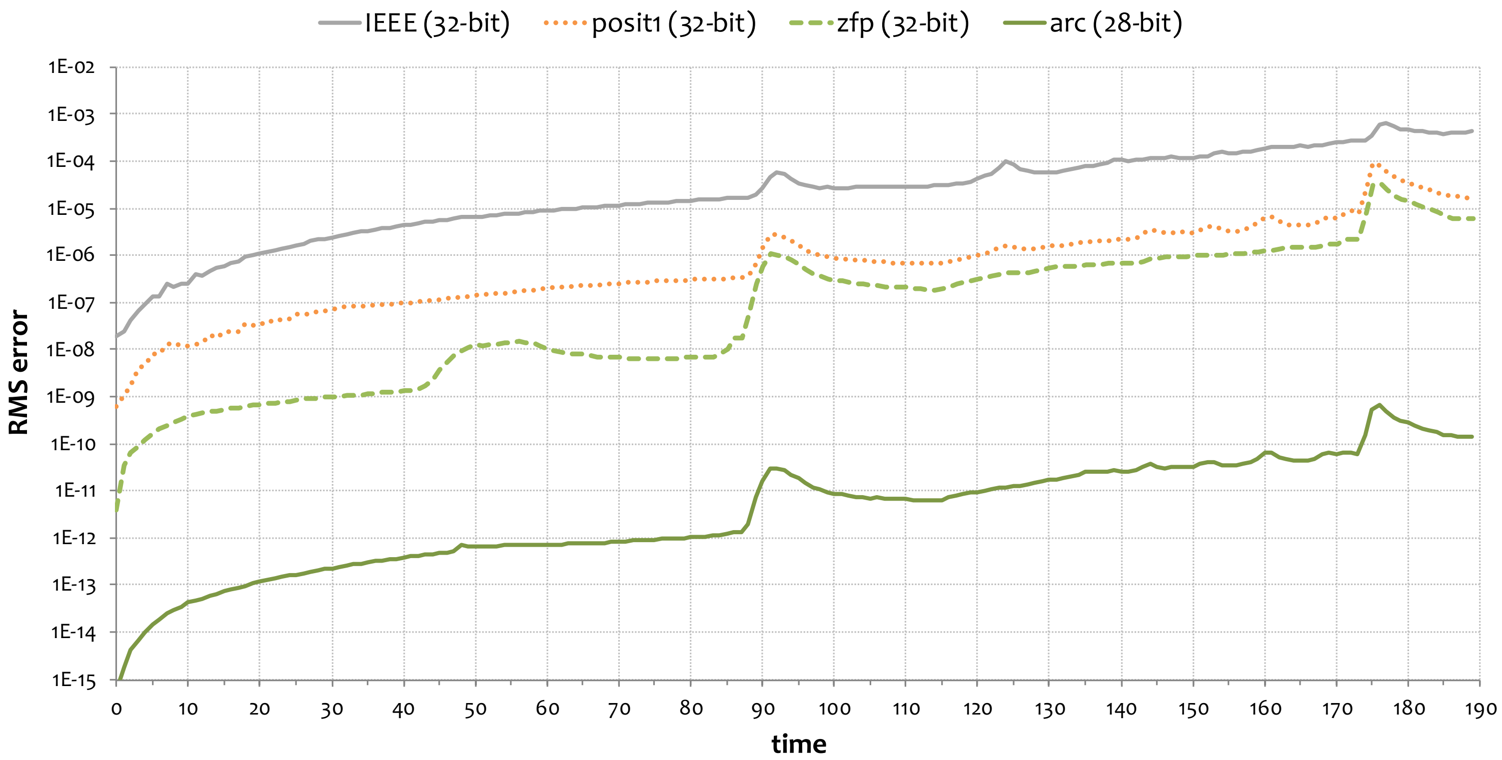
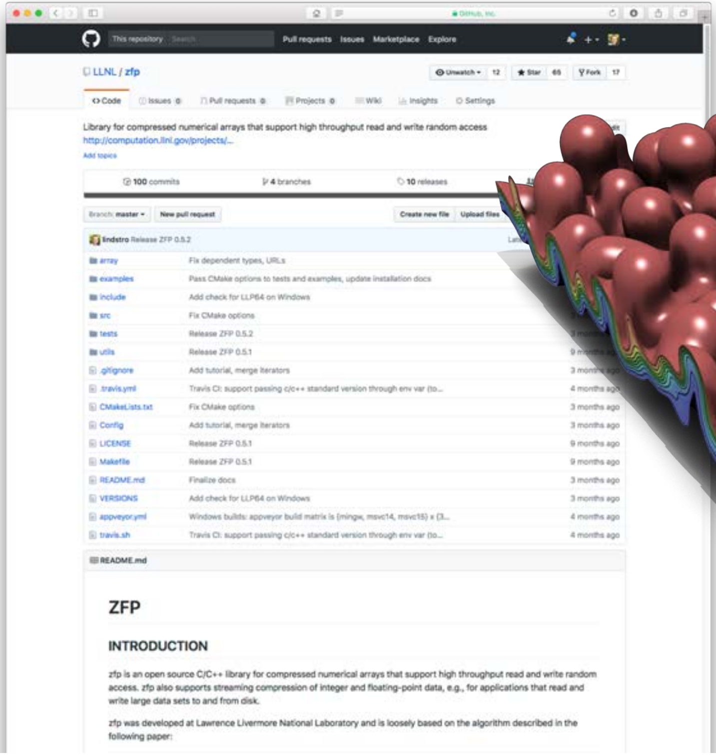
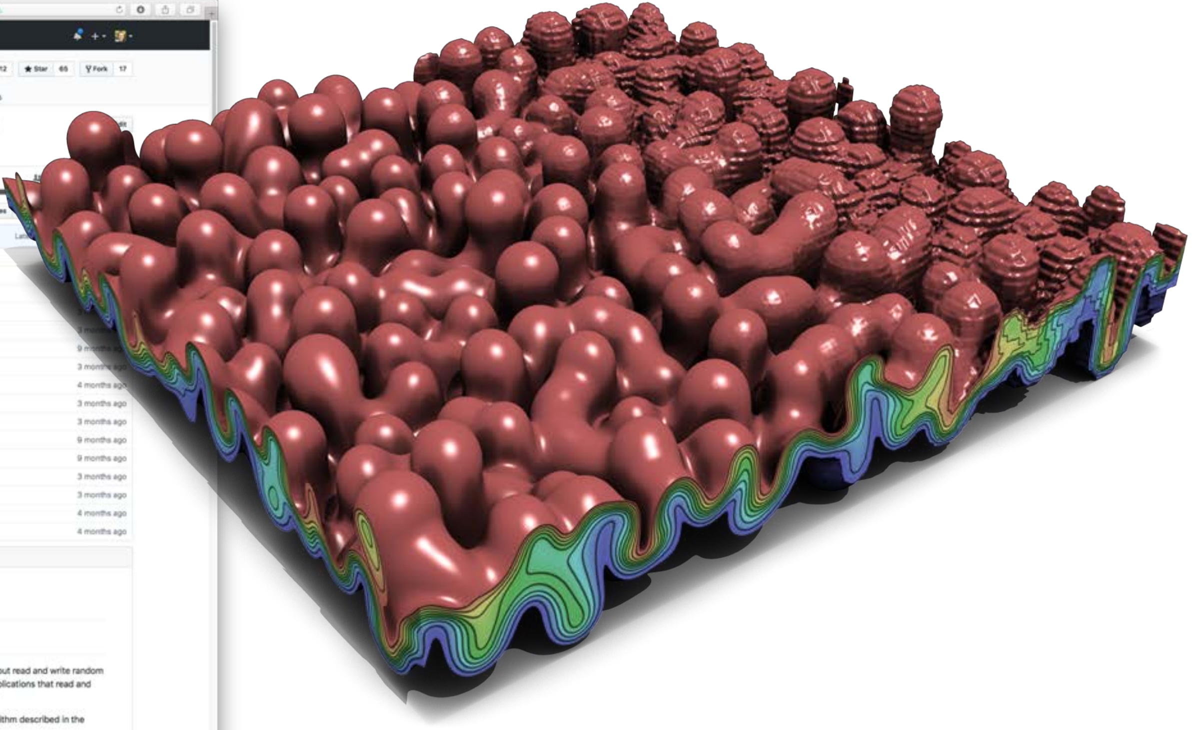


Conclusions: Novel scalar representations are driving research into new vector/matrix/tensor representations

- Emerging alternatives to IEEE floats show promising improvements in accuracy
  - **Tapered precision** allows for better balance between range and precision
  - New types have many desirable properties
    - No IEEE warts: *subnormals*, *excess of NaNs*, *signed zeros*, *overflow*, *exponent size dichotomy*, …
    - Features: *nesting*, *monotonicity*, *reciprocal closure*, *universality*, *asymptotic optimality*, …
- NumRep framework allows for experimentation with new number types in apps
  - **Modular design** supports plug-and-play of independent concepts
  - **Nonlinear maps** are expensive but worth investigating
  - POSITS are often among the best performing types; IEEE among the worst
- NextGen scalar representations still leave considerable room for improvement
  - ZFP fixed-rate compressed arrays consistently outperform IEEE and POSITS
  - ZFP **variable-rate arrays** optimize bit distribution and and **make very bit count**

ZFP is available as open source on GitHub: https://github.com/LLNL/zfp





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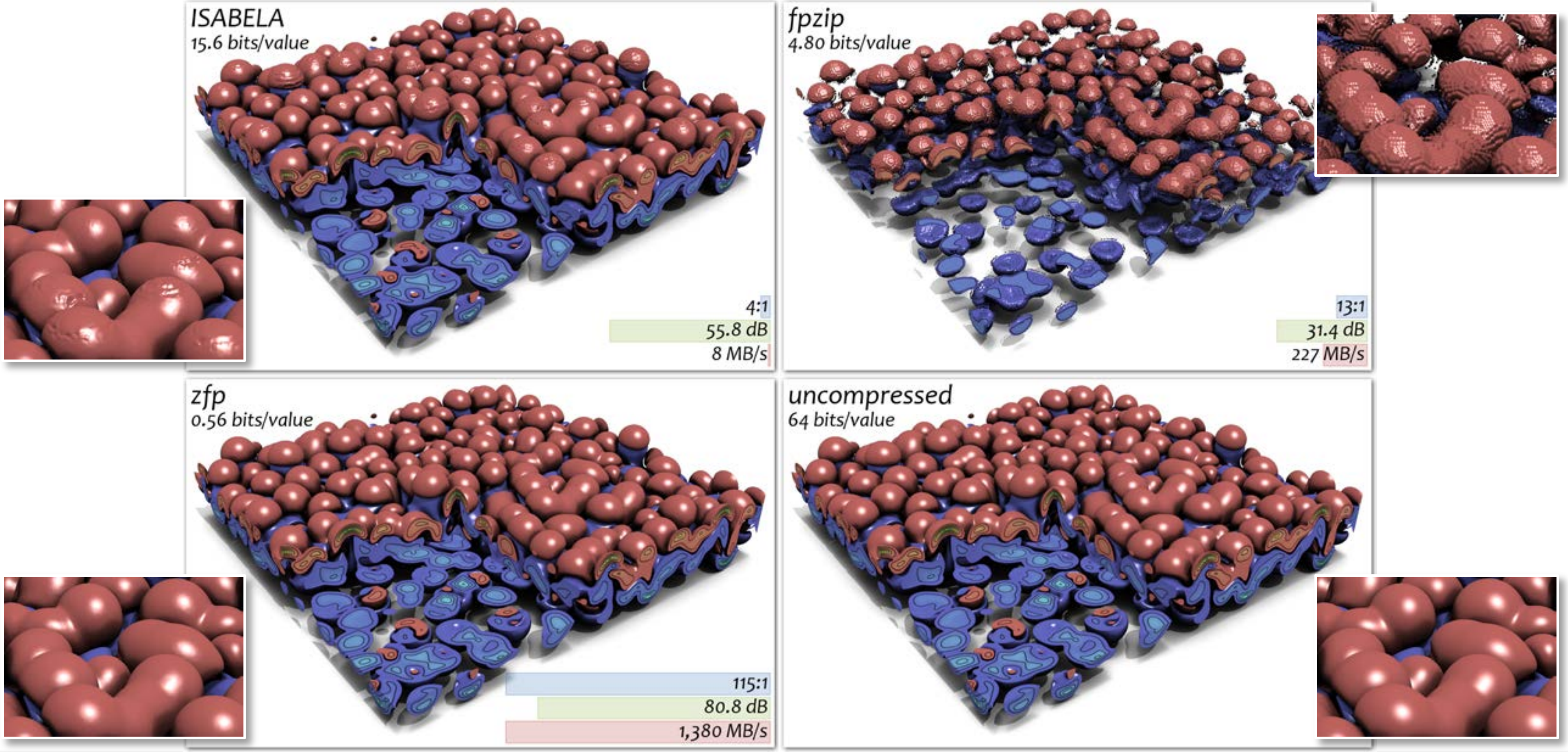
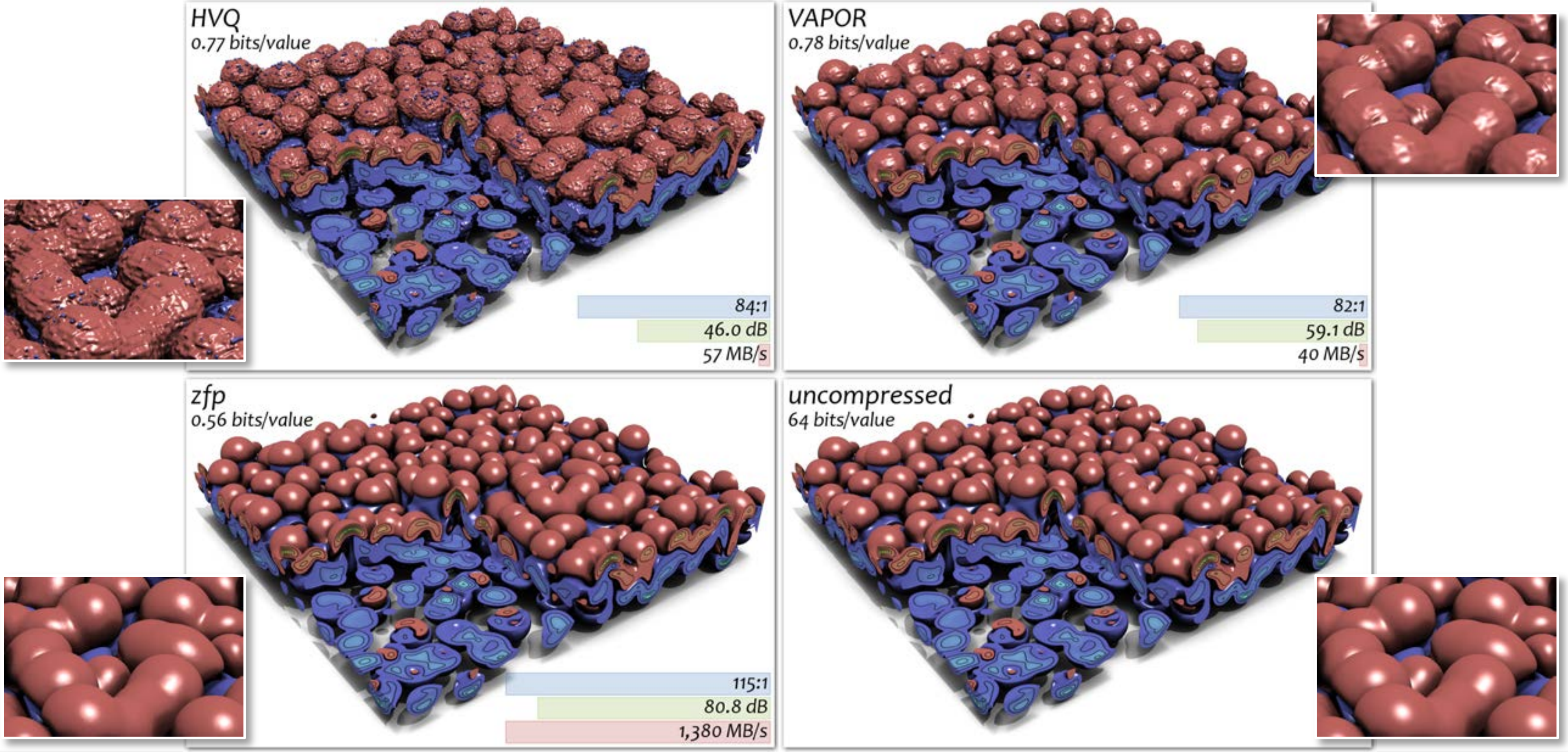
ZFP provides >100x compression with imperceptible loss in visual quality



ZFP provides >100x compression with imperceptible loss in visual quality



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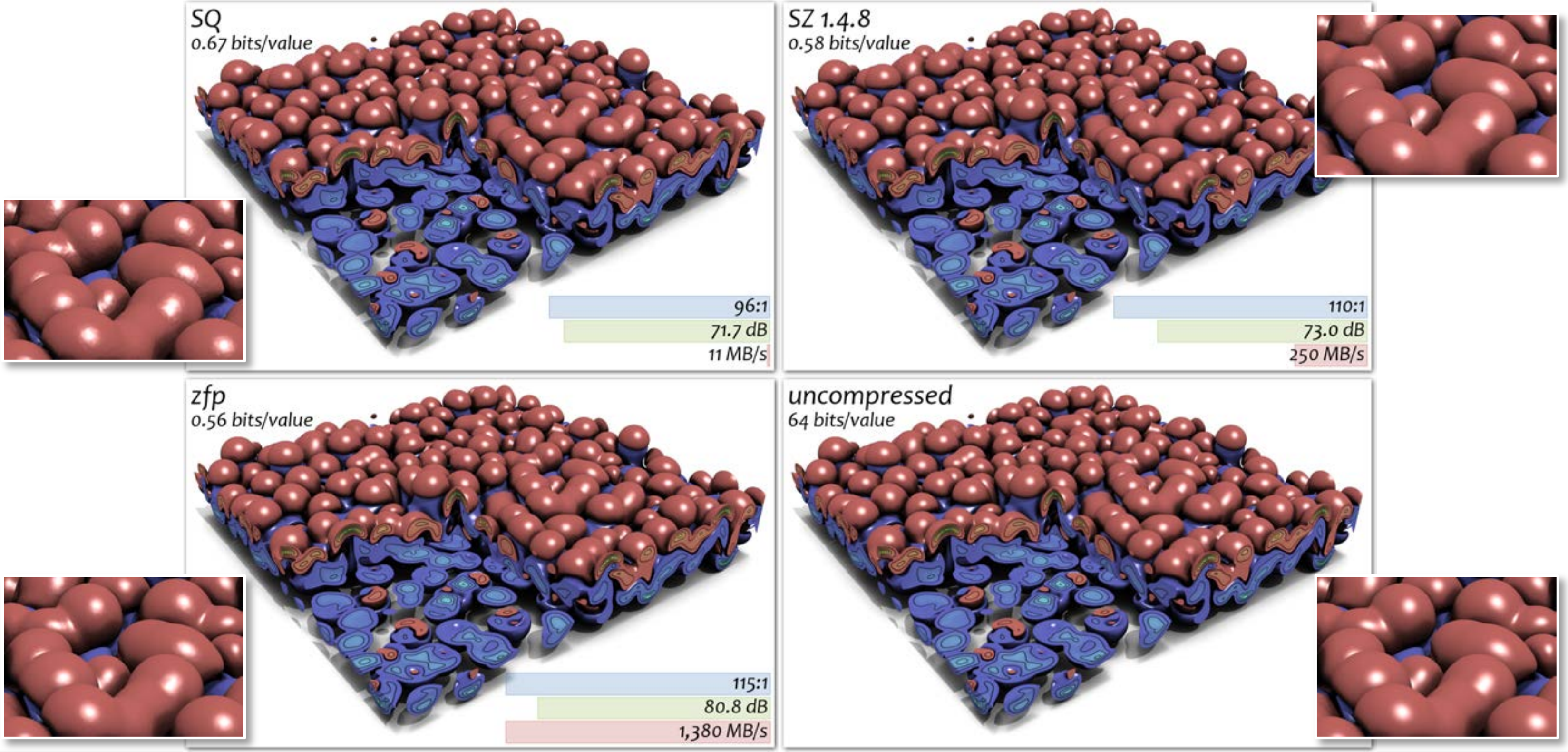
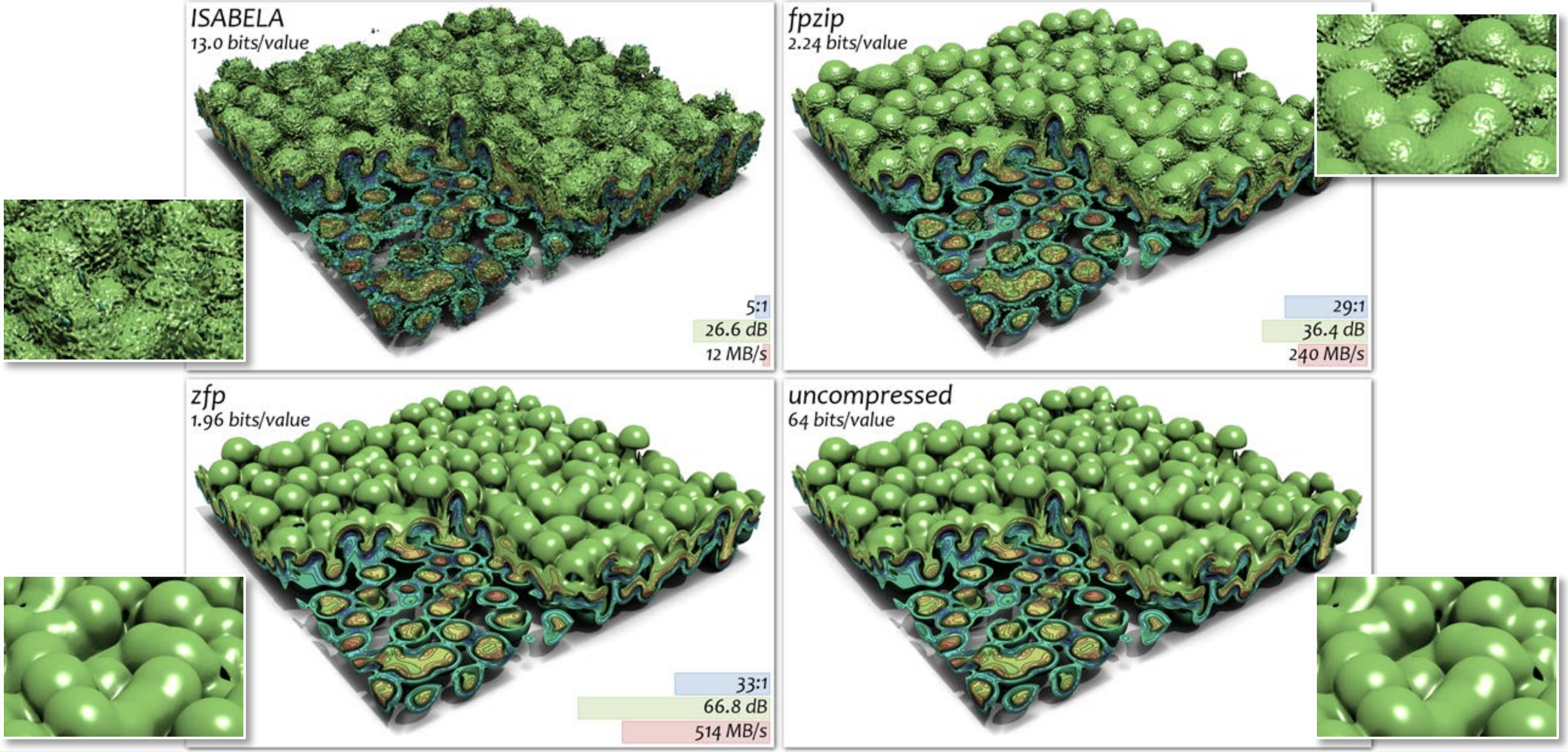


ZFP shows no artifacts in derivative computations (velocity divergence)



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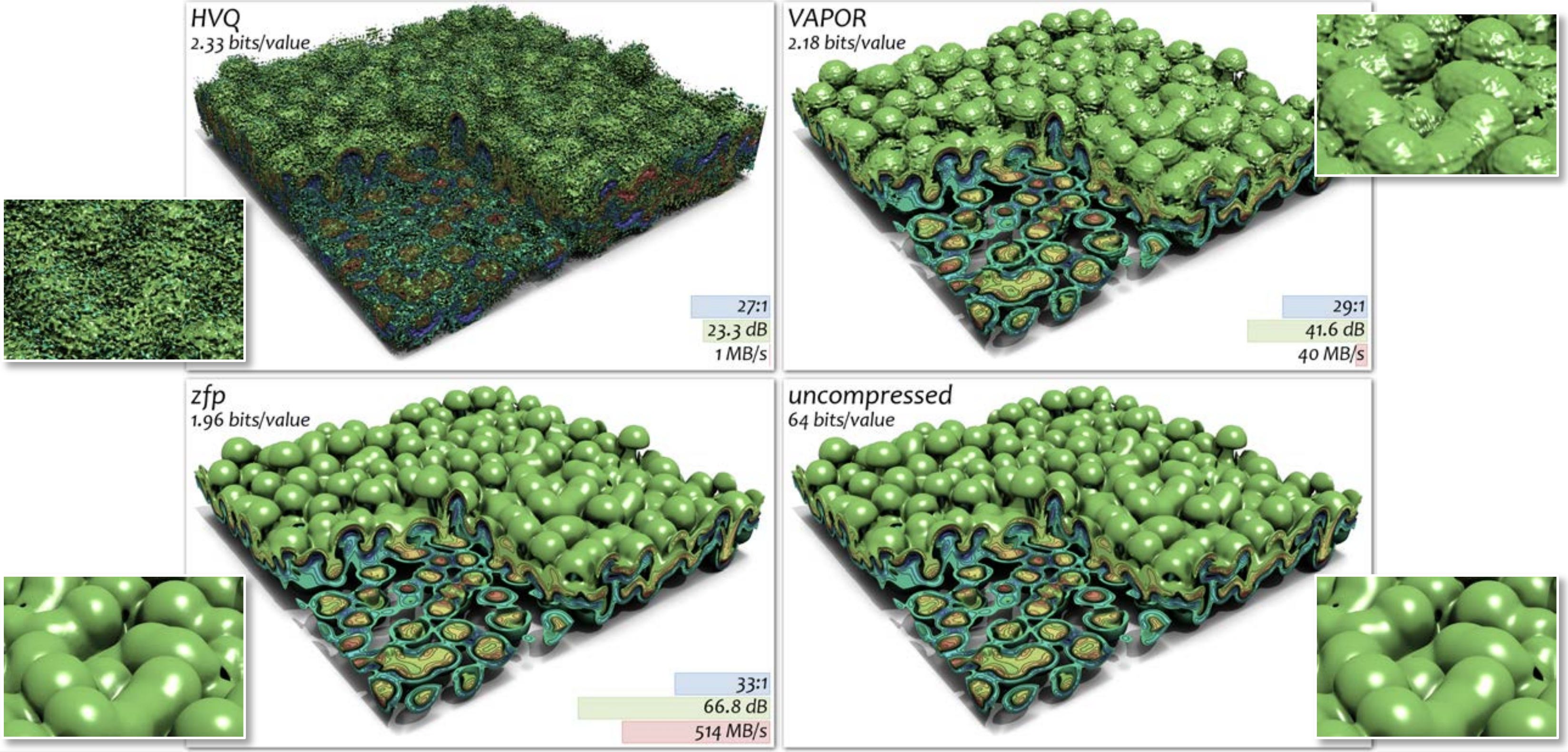

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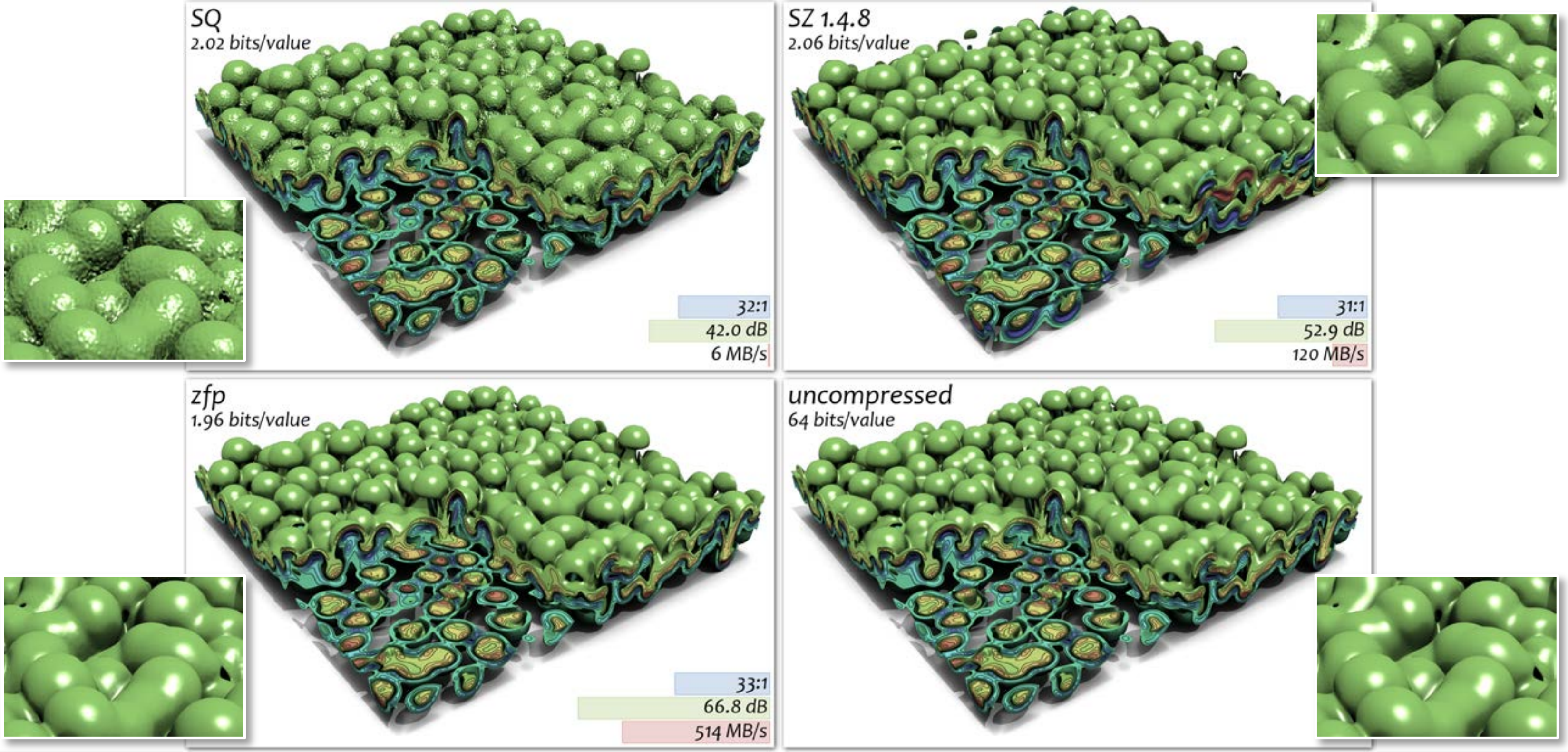

Parallel ZFP achieves up to 150 GB/s throughput