

Direct Measurement of Numerical Accuracy

Cédric Chevalier, CEA, DAM, DIF

Floating point computations and correctness

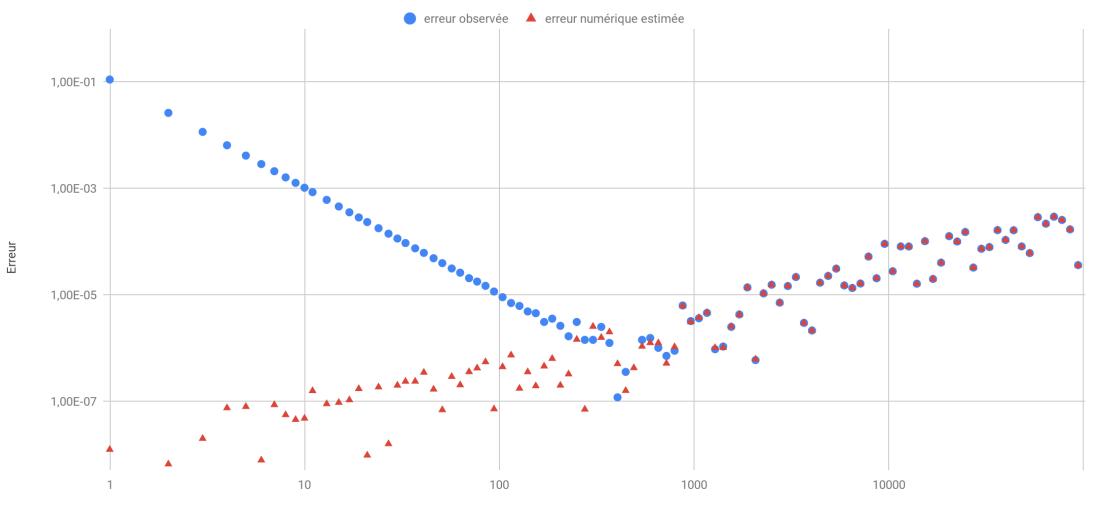
- Most of Kokkos applications performs floating point computations
- And they care about their results
- Several related questions
 - How to unit tests numerical applications if outputs are allowed to change
 - New hardware
 - New software
 - Non deterministic computations
 - What floating point representation is the most efficient for my use case (float vs double vs AI)
- We (the CExA project) are currently porting Shaman (<u>https://gitlab.com/numerical_shaman/shaman</u>), a numerical profiler to Kokkos ecosystem

Numerical Integration: Rectangle Method



π/2

How accurate are we?



Nombre de rectangles



CG Convergence vs Rounding Errors



conditionnement de la matrice

Classical Algorithm (Trilinos/Belos):

Error distribution: [matrix_vector_product:99%...]

Iterations: 5000 Residual: 3400 Not converged

Compensated matrix-vector product Error distribution: [dot_product1:94%...]

Iterations: 1494 Residual: 0.8 « Converged »

The Idea Behind Shaman



We introduce a new datatype that stores the original value and operation errors

Errors are propagated and computed using Error Free Transforms

```
Snum operator+(Snum n1, Snum n2)

{

numberType result = n1.number + n2.number;

numberType errorOperator = EFT::TwoSum(n1.number, n2.number);

errorType newError = errorOperator + (n1.error + n2.error);

return Snum(result, newError);

};

double TwoSum(double x, double y)

{

double result = x + y;

double x2 = result - x;

double x2 = result - y2;

double epsilon1 = y - y2; // ≠ 0

double epsilon2 = x - x2; // ≠ 0

double error = epsilon1 + epsilon2;

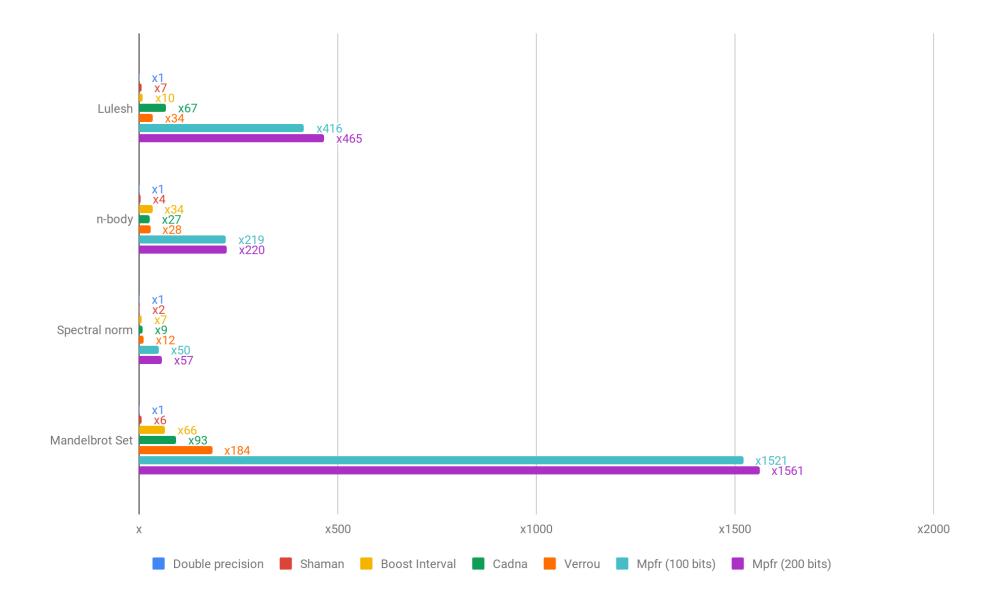
return error;

};
```

Main expected issue when going to Kokkos:

how to ensure that compilers will not optimize out useful computations.

CPU Performance





Thank you !

CEA, DAM, DIF Arpajon France

Phone. + 33 1 69 26 40 00

