Improving Numerical Reproducibility in C/C++/Fortran

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Code the Future
The Three Objectives

• Accuracy
• Reproducibility
• Performance

Pick two
Reproducibility

Consistent results:

• From one run to the next
• From one set of build options to another
• From one compiler (or compiler version) to another
• From one processor or operating system to another
Factors that affect reproducibility

- Floating-point semantics
- Use of higher-precision intermediate results
- Differences in math libraries
- Optimization choices
- Parallelism changing operation order
- Data alignment changing vectorization
- Implementation differences between processors

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Floating-Point Semantics

Compiled code transformations that may not be value-safe

• Reassociation – \((x+y)+z\) to \(x+(y+z)\)
• Divide using multiply by reciprocal
• Underflow to zero
• Constant-folding
• Keeping higher precision
Reassociation

• Addition and multiplication are mathematically associative, but not computationally associative

• C and C++ disallow reassociation, specify left-to-right order

• Fortran allows reordering as long as parentheses are honored

• Compiler may not obey these by default
Optimization and Instruction Sets

• Affects order of operations and grouping of intermediate results
• Newer instruction sets enable more vectorization
• Fused multiply-add different from separate
• Automatic CPU dispatch in math libraries can change results
Data Alignment

- Misaligned data requires prefix and postfix loop plus main vectorized loop body
- Can change results run-to-run!
  - OS stack alignment
  - Address Space Layout Randomization
CAM (Community Atmospheric Model) example

A(I) + B + TOL

where

• TOL was very small and positive
• A(I) and B could be large

Compiler evaluated this as A(I) + (B + TOL)

Hoisted constant B + TOL out of the loop

TOL got rounded away....
Example

do i=1,10000
    sum = sum + sqrt(values(i))
end do

No optimization: 0.2919665E+08
With optimization: 0.2919677E+08
With advanced instructions: 0.2919678E+08
Misaligned data: 0.2919677E+08
Double precision: 0.29196781789902E+08
What can you do?

- Examples from Intel Fortran
- Other compilers may have similar options
What can you do?

- Align data to vector register width (512 bits for current Intel architectures)
  - !DIR$ ATTRIBUTES ALIGN
  - !DIR$ VECTOR_ALIGNED
  - !DIR$ ASSUME_ALIGNED
  - -align
- Use parentheses liberally
  - Intel Fortran – add –assume protect_parens
The -fp-model (/fp:) switch lets you choose the floating point semantics at a coarse granularity. It lets you specify the compiler rules for:

- Value safety
- FP expression evaluation
- FPU environment access
- Precise FP exceptions
- FP contractions
-fp-model

- fast [=1] allows value-unsafe optimizations (default)
- fast=2 allows additional approximations
- precise value-safe optimizations only (also source, double, extended)
- except enable floating point exception semantics
- strict precise + except + disable fma
FP Expression Evaluation

• $a = (b + c) + d$

• Four possibilities for intermediate rounding, (corresponding to C99 FLT_EVAL_METHOD)
  • Indeterminate (-fp-model fast)
  • Use precision specified in source (-fp-model source)
  • Use double precision (C/C++ only) (-fp-model double)
  • Use long double precision (C/C++ only) (-fp-model extended)
  • Or platform-dependent default (-fp-model precise)

• The expression evaluation method can significantly impact performance, accuracy, and portability!

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Value Safety

• In SAFE (precise) mode, the compiler may not make any transformations that could affect the result, e.g. the following is prohibited:
  
  \[(x + y) + z \rightarrow x + (y + z)\]

  general reassociation is not value safe

• UNSAFE (fast) mode is the default
  
  • The variations implied by “unsafe” are usually very tiny

• VERY UNSAFE (fast=2) mode enables riskier transformations

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Reductions

- Parallel implementations imply reassociation (partial sums)
  - Not value safe
  - -fp-model precise
    - disables vectorization of reductions
    - does not affect OpenMP\* or MPI\* reductions
  - These remain value-unsafe (programmer’s responsibility)
What can you do?

- **-fp-model** *keyword* (fast, precise, except, strict, source)
- **-fimf-arch-precision**=(high, medium, low) – controls accuracy of math library functions
- **-fimf-arch-consistency**=true – Math library gives same results across processors
- **KMP_DETERMINISTIC_REDUCTION**=1 for OpenMP reductions
Summary

• Reproducibility is a tradeoff against accuracy and performance
• Decide which kinds of reproducibility are important to you
• There are things you can do to help reduce differences
References

Consistency of Floating-Point Results using the Intel® Compiler (Martyn Corden and David Kreitzer) [http://intel.ly/1eiQxua](http://intel.ly/1eiQxua)

Differences in Floating-Point Arithmetic Between Intel® Xeon® Processors and the Intel® Xeon Phi™ Coprocessor (Corden) [http://intel.ly/1b8Qrq6](http://intel.ly/1b8Qrq6)

Optimization Notice

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