Interval Arithmetic Support In The Fortran Compiler

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This Is Not A Scientific Talk
Outline

- Introduction
- Interval-Specific Operators and Intrinsic Functions
- Quality Of Implementation Opportunities
- Conclusions
Good News For Intervals!

- Sun has been awarded the DARPA HPCS contract
  - HPCS = High Productivity Computing Systems
  - HPCS Goal: Build a Peta-scale system
  - This is phase 2 of a 3-tier project
  - Three vendors selected (IBM, Cray and Sun)

- One key element in Sun's proposal is the usage of [ Inter, vals ]
Introduction

- This presentation is based on discussions with Bill Walster (Sun Microsystems)
  - Without his relentless enthusiasm there would not have been an interval compiler from Sun
  - An extensive interview with Bill can be found at http://www.sun.com/presents/minds/2004-0527

- The Sun Fortran and C++ compilers support intervals since 2000 (available on SPARC based systems)
  - Fortran: native data type
  - C++: class library

- In this talk we would like to give an overview of the interval features supported in the Sun Fortran compiler
Pointers To More Information/1

- **Download the compilers (Sun Studio 8)**
  - **URL is** [http://developers.sun.com/prodtech/cc](http://developers.sun.com/prodtech/cc)
  - **Can use a free “try and buy” license and/or**
  - **Interval support (Fortran and C++) included**

  ✔️ **Use -xia option to activate**
Pointers To More Information/2

- **Documentation**
  - *Fortran Interval Arithmetic Programming Reference*
    - [http://docs.sun.com/db/doc/817-5076](http://docs.sun.com/db/doc/817-5076)
  - *C++ Interval Arithmetic Programming Reference*
    - [http://docs.sun.com/db/doc/817-5077](http://docs.sun.com/db/doc/817-5077)

- **More information plus code examples can be downloaded from** [http://developers.sun.com](http://developers.sun.com)
  - Go to the “Compiler Collection” portal

- **Another useful web site (on numerical computations):**
  - [http://developers.sun.com/prodtech/cc/numerics_index.html](http://developers.sun.com/prodtech/cc/numerics_index.html)
Basic Interval Arithmetic
Basic Arithmetic Operations

Assume that \([a,b]\) and \([c,d]\) are intervals

For a basic operator "op" in \{+,-,\*,/\} we can then define:

\[ [a,b] \ "op" \ [c,d] \supseteq \{x \ "op" \ y \mid x \in [a,b] \text{ and } y \in [c,d]\} \]

Formulas for basic operations:

\[
\begin{align*}
[a,b] + [c,d] &= [a+c,b+d] \\
[a,b] - [c,d] &= [a-d,b-c] \\
[a,b] \times [c,d] &= [\min(a*c,a*d,b*c,b*d), \max(a*c,a*d,b*c,b*d)] \\
[a,b] / [c,d] &= [\min(a/c,a/d,b/c,b/d), \max(a/c,a/d,b/c,b/d)] \\
&\quad (\text{if } 0 \text{ is not included in } [c,d])
\end{align*}
\]
Interval-Arithmetic Applications
Types of problems

- Unconstrained Global nonlinear minimization
- Constrained Global nonlinear minimization
- Guaranteed equation solving
- Imaging of a set by nonlinear function
Types of problems

- Probably the most current source for applications is the Proceedings of the NSF Workshop on Reliable Engineering Computing, held in November, 2004 at the Georgia Institute of Technology. See:
  
  <http://www.gtsav.gatech.edu/rec/recworkshop/>

- Papers on mechanical and chemical engineering. There has been a lot of excellent work on integrating ODEs.
  
  <http://www.bt.pa.msu.edu/cgi-bin/displaytest.pl?name=VIRC03>

- The use of Taylor multinomials and arithmetic on them has been used to solve particle-beam accelerator design problems. See:
  
  <http://www.bt.pa.msu.edu/index_files/cosy.htm>
F95 Interval Support Goal
F95 interval support Goal

- Quality interval code
- Narrow-width interval results
- Rapidly executing interval code
- An easy to use interval software development environment that includes interval-specific language support and compiler features

This will stimulate interval solver libraries and applications
Narrow-Width Interval Results

- Minimize the width of computed intervals while always satisfying the containment constraint.
- If an interval's width is as narrow as possible, it is said to be sharp.
- Width of intervals produced by the f95 compiler:
  - Individual intervals are sharp approximations of constants.
  - Individual interval arithmetic operators produce sharp results.
  - Intrinsic mathematical functions usually produce sharp results.
Easy to Use Development Environment

- **INTERVAL data types**
- **INTERVAL arithmetic operations and intrinsic mathematical functions form a closed mathematical system.**
- **Intrinsic INTERVAL-specific operators, such as .IX. (intersection) and .IH. (interval hull)**
- **INTERVAL-specific functions, such as INF, SUP, and WID**
- **Three classes of interval relational operators:**
  - Certainly
  - Possibly
  - Set
Command Line Options

- **Compiler support for widest-need interval expression processing is invoked by including:**
  - `-xia` or `-xia=widestneed`

- **Compiler support for strict interval expression processing is invoked by including:**
  - `-xia=strict`
Interval-Specific Operators and Intrinsic Functions
Basic Arithmetic Operations

Assume that \([a,b]\) and \([c,d]\) are intervals.

For a basic operator "op" in \{+,−,∗,\}/\ we can then define:

\[
[a,b] \text{ "op" } [c,d] \supseteq \{ x \text{ "op" } y | x \in [a,b] \text{ and } y \in [c,d] \}
\]

Formulas for basic operations:

\[
\begin{align*}
[a,b] + [c,d] &= [a+c, b+d] \\
[a,b] - [c,d] &= [a-d, b-c] \\
[a,b] \times [c,d] &= [\min(a*c, a*d, b*c, b*d), \\
&\quad \max(a*c, a*d, b*c, b*d)] \\
[a,b] / [c,d] &= [\min(a/c, a/d, b/c, b/d), \\
&\quad \max(a/c, a/d, b/c, b/d)]
\end{align*}
\]

(if 0 is not included in \([c,d]\))
Integer Powers

The Dependence Problem:

\([-1, 2] \times [-1, 2] = [-2, 4]\]

The Sun Compiler will do the right thing:

```f95
% f95 -o pow -xia pow.f95
% ./pow
X     = [ -1.00000000,  2.00000000]
X*X    = [ -2.00000000,  4.00000000]
X**2   = [  0.00000000,  4.00000000]
```
Order Relations - What To Do?

- [a, b] certainly less than [c, d]
- [a, b] possibly less than [c, d]

Implementation in the Sun compiler:
One of \{C, P, S\}, followed by LT/LE/EQ/NE/GE/GT

Example: A .CLT. B
### Set-Theoretic Interval Operators

<table>
<thead>
<tr>
<th>Name</th>
<th>Math. Notation</th>
<th>Fortran</th>
<th>Result Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interval hull</td>
<td>$X \cup Y$</td>
<td>$X.IH.Y$</td>
<td>Interval</td>
</tr>
<tr>
<td>Intersection</td>
<td>$X ? Y$</td>
<td>$X.IX.Y$</td>
<td>Interval</td>
</tr>
<tr>
<td>Disjoint</td>
<td>$X ? Y = \emptyset$</td>
<td>$X.DJ.Y$</td>
<td>Logical</td>
</tr>
<tr>
<td>Element</td>
<td>$r \in Y$</td>
<td>$R.IN.Y$</td>
<td>Logical</td>
</tr>
<tr>
<td>Interior</td>
<td>$X &lt; Y \text{ and } \overline{X} &lt; Y$</td>
<td>$X.INT.Y$</td>
<td>Logical</td>
</tr>
<tr>
<td>Proper subset</td>
<td>$X \subset Y$</td>
<td>$X.PSB.Y$</td>
<td>Logical</td>
</tr>
<tr>
<td>Proper superset</td>
<td>$X \supset Y$</td>
<td>$X.PSP.Y$</td>
<td>Logical</td>
</tr>
<tr>
<td>Subset</td>
<td>$X \subseteq Y$</td>
<td>$X.SB.Y$</td>
<td>Logical</td>
</tr>
<tr>
<td>Superset</td>
<td>$X \supseteq Y$</td>
<td>$X.SP.Y$</td>
<td>Logical</td>
</tr>
</tbody>
</table>
All Fortran intrinsic functions have an interval counterpart if they either return a REAL, or accept a REAL type argument

% cat -n cos.f95
1    program demo
2
3 print *, 'cos (-0.5) = ', cos(-0.5D0)
4 print *, 'cos (+0.5) = ', cos(+0.5D0)
5 print *, 'cos [-0.5,+0.5] = ', cos([-0.5,+0.5])
6
7 stop
8 end

% f95 -o cos -xia cos.f95
% ./cos

cos (-0.5) = 0.8775825618903728

cos (+0.5) = 0.8775825618903728

cos [-0.5,+0.5] = [0.87758256189037264, 1.0]
## Interval Specific Intrinsicics

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Name</th>
<th>Result Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>Infimum</td>
<td>$\inf([a,b]) = a$</td>
<td>INF</td>
<td>REAL</td>
</tr>
<tr>
<td>Supremum</td>
<td>$\sup([a,b]) = b$</td>
<td>SUP</td>
<td>REAL</td>
</tr>
<tr>
<td>Width</td>
<td>$w([a,b]) = b-a$ ((a+b)/2)</td>
<td>WID</td>
<td>REAL</td>
</tr>
<tr>
<td>Midpoint</td>
<td>$\max(</td>
<td>a</td>
<td>,</td>
</tr>
<tr>
<td>Magnitude</td>
<td>$\max(</td>
<td>a</td>
<td>,</td>
</tr>
<tr>
<td>Magnitude</td>
<td>$\min(</td>
<td>a</td>
<td>,</td>
</tr>
<tr>
<td>Empty Test</td>
<td>TRUE if empty</td>
<td>ISEMPTY</td>
<td>LOGICAL</td>
</tr>
<tr>
<td>Number Of Digits</td>
<td>Max. digits</td>
<td>NDIGITS</td>
<td>INTEGER</td>
</tr>
</tbody>
</table>

* ) Returns 0 if $0 \in [a,b]$
Input / Output

- Square brackets ("[ " and "]") are used to delimit intervals
  - Example: $X = [-0.1, 0.2]$
- All edit descriptors that accept REAL data items also accept INTERVAL data
- Specific INTERVAL edit descriptors are supported as well
Quality Of Implementation Opportunities
Supported Features

- A closed interval system in which all expressions (including singularities and indeterminate forms) are defined
  - Examples: 1/0, \(x^y\) with \(x=y=0\), operations involving \(+\infty\) and/or \(-\infty\)

- Domain constraints on intrinsic functions are gracefully handled
  - Example: \(\text{SQRT}([-1, +1]) = [0, 1]\)

- Input / Output can be handled in different ways

- Context dependent literal interval constants

- Mixed mode expressions
Example Code

Program Demo
logical :: not_done = .true.
interval(kind=8) :: ai, bi
write(*,*) 'Please give values for A and B'
do while ( not_done )
    read(*,*,end=9000) ai, bi
    write(*,9010) '+',ai,'+',bi,ai+bi
    write(*,9010) '-',ai,'-',bi,ai-bi
    write(*,9010) '*',ai,'*',bi,ai*bi
    write(*,9010) '/',ai,'/',bi,ai/bi
end do

9000 continue
9010 format(1X,'A',1X,(A),1X,'B =',VF17.4,1X,(A), & 1X,VF17.4,' = ',VF17.4)
end
Example Closed Interval System

Please give values for A and B

\[ A + B = [-1.0000, 3.0000] + [1.0000, 2.0000] = [0.0000, 5.0000] \]
\[ A - B = [-1.0000, 3.0000] - [1.0000, 2.0000] = [-3.0000, 2.0000] \]
\[ A \times B = [-1.0000, 3.0000] \times [1.0000, 2.0000] = [-2.0000, 6.0000] \]
\[ A / B = [-1.0000, 3.0000] / [1.0000, 2.0000] = [-1.0000, 3.0000] \]

\[ A + B = [1.0000, 2.0000] + [-1.0000, 3.0000] = [0.0000, 5.0000] \]
\[ A - B = [1.0000, 2.0000] - [-1.0000, 3.0000] = [-2.0000, 3.0000] \]
\[ A \times B = [1.0000, 2.0000] \times [-1.0000, 3.0000] = [-2.0000, 6.0000] \]
\[ A / B = [1.0000, 2.0000] / [-1.0000, 3.0000] = [-\text{Inf}, \text{Inf}] \]
Summary

- The Sun Fortran and C++ compilers support Interval Arithmetic
- The regular Basic Arithmetic Operations, intrinsic functions and logical operations have been extended to intervals
- In addition to this, several quality of implementation features are supported:
  - Closed interval system, domain constraints on intrinsic functions, input/output, context dependent literal interval constants, etc.
- We believe that this provides for a production quality interval compiler
We Need Your Help

For Sun to continue interval support, we need you to use our compilers and give feedback

Feel free to send me an email: sambath.narayanan@sun.com
Thank You!
Why Is Interval Arithmetic Important?

- *Interval arithmetic can be used to perform machine computations with guaranteed bounds on errors from all sources, including input data errors, machine rounding errors, and their interactions.*

- *Interval algorithms can be used to solve nonlinear problems, such as the solution to nonlinear systems of equations and nonlinear programming (the nonlinear extension to linear programming).*

- *As intervals become more widely used, libraries of interval solvers will be used routinely to compute sharp (narrow width) interval solutions to linear and nonlinear problems, while taking into account all sources of error. With these libraries, scientists, engineers, and developers of commercial applications will be able to write programs to solve problems that are currently beyond reach.*
Support for intrinsic `INTERVAL` data types is a feature in the Sun WorkShop 6 Fortran 95 compiler. Two new compiler flags, `-xia` and `-xinterval`, tell the compiler to recognize interval-specific language extensions and to generate executable interval code.

The Sun WorkShop 6 C++ compiler provides a C++ interface to the C++ interval arithmetic library. To use the C++ interval arithmetic features, add the `#include <suninterval.h>` header file to the code, and then compile the code using the `-xia` command-line option.
Beam Dynamics

- *beam dynamics simulation and analysis code*. It allows the study of accelerator lattices, spectrographs, beamlines, electron microscopes, and many other devices. It can determine high-order maps of combinations of particle optical elements of arbitrary field configurations. The elements can either be based on a large library of existing elements with realistic field configurations including fringe fields, or described in detail by measured data.

- Analysis options include computation of high-order nonlinearities; analysis of properties of repetitive motion via chromaticities, normal form analysis, and symplectic tracking; analysis of single-pass systems resolutions, reconstructive aberration correction, and consideration of detector errors; and analysis of spin dynamics via computation of spin maps, spin normal form and spin tracking.