ECMWF Workshop on High Performance Computing in Meteorology

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Agenda

• Company Overview

• Rogue Wave Product Overview
  – IMSL Fortran
  – TotalView Debugger
  – Acumem ThreadSpotter
Rogue Wave

- **History**
  - Founded: 1989
  - Named after the founder’s boat
  - Acquisitions:
    - Visual Numerics: 2009
    - TotalView Technologies: 2010
    - Acumem: 2010

- **Global Locations**
  - HQ: Boulder, CO
  - NA: Houston, TX; Corvallis, OR; Natick MA
  - EMEA: France, Germany, Sweden, UK
  - APAC: Japan

- **Customers**
  - 3,000+ in 36 countries
  - Financial services, telecoms, oil and gas, government and aerospace, research and academic
Rogue Wave Today

The largest independent provider of cross-platform software development tools and embedded components for the next generation of HPC applications

Leading provider of enterprise class C++ components and infrastructure for high performance applications.

Visual Numerics
Leader in embeddable math and statistics algorithms and visualization software for data-intensive applications.

TotalView Technologies
Industry-leading interactive analysis and debugging tools for the world's most sophisticated software applications.

Scumem
Leading provider of intelligent software technology which analyzes and optimizes the computing performance in single- and multi-core environments.
Agenda

- Company Overview
- Rogue Wave Product Overview
  - IMSL Fortran
    - CUDA support
  - TotalView Debugger
    - Remote Display Client
    - TVScript for Batch Debugging
    - MemoryScape and ReplayEngine
  - Acumem ThreadSpotter
Rogue Wave Product Family

PROTOTYPE ë DEVELOP ë DEBUG ë OPTIMIZE
IMSL Fortran Library

Now supports NVIDIA GPUs
Parallelism Using the IMSL Fortran Library

- **OpenMP**
  - Linear systems, Eigensystem Analysis, Transforms, etc.
  - The corresponding routines differ by environment
  - IMSL uses the OpenMP directive to parallelize internally; users do not need to write parallel program source

- **MPI**
  - Linear Algebra Operator and Generic Function, Linear systems, etc.
  - Corresponding routines are the same in all environments
  - Users need to call the IMSL function MP_SETUP()
IMSL Fortran Library 7.0

• Integration of NVIDIA CUDA BLAS
  – Support NVIDIA GPU hardware (Tesla, Fermi)
  – Call CUDA Level 2 and 3 BLAS functions
    • Problem size must be large enough to see the benefit
    • Use IMSL functions as usual, calls NVIDIA’s library behind the scenes
    • If no GPU hardware or smaller problem, execute on CPU
  – Double and Single precision
  – Benchmark white paper available
    http://www.vni.com/products/imsl/fortran/
Throughput Results

Times for Array Size of 500

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- SGEMM
- DGEMM
- CGEMM
- ZGEMM

Legend:
- Fortran
- Vendor 1 Core
- Vendor 4 Core
- NVIDIA
Throughput Results (cont.)

Times for Array Size of 4000

- SGEMM
- DGEMM
- CGEMM
- ZGEMM

Legend:
- Fortran
- Vendor 1 Core
- Vendor 4 Core
- NVIDIA
TotalView Debugging Technology

• What is TotalView?
  – Parallel and Multithreaded Debugging and Analysis Tool
  – For scientists and engineers working with C/C++ and Fortran
  – Makes developing, maintaining and supporting critical and cutting edge applications easier and less risky

• Major Features
  – Supports Linux, Unix and Mac OS X
  – Parallel Debugging
    – MPI, Pthreads, OMP, UPC
  – Includes a Remote Display Client freeing users to work from anywhere
  – Memory Debugging with MemoryScape
  – Optional Reverse Debugging with ReplayEngine
  – Batch Debugging with TVScript and the CLI

• Advantages
  – Easy to learn graphical user interface with data visualization
  – Wide variety of features so users can tackle unexpected bugs
  – Consistent functionality and look and feel across a wide range of platforms
  – Works robustly with open source and vendor compilers
  – Native debugger core is highly scalable to large clusters, large code and massive datasets
How can TotalView help you?

Debugging means examining a specific controlled instance of program execution
Provides an answer to the question: “What is my program really doing?”

- **Threads and/or MPI**
  - When you have
    - Deadlocks and hangs
    - Race conditions
  - It provides
    - Asynchronous thread control
    - Barrier points
    - Powerful group mechanism

- **Fortran and/or C++**
  - Complex data structures
    - Diving and recursive dive
  - STL Collection Classes
    - STLView
  - Rich class hierarchies
    - Powerful type-casting features

- **Memory Analysis**
  - Leaks and Bounds Errors
    - Automatic error detection tools
  - Out of Memory Errors
    - Analysis of heap memory usage by file function and line

- **Data Analysis**
  - Numerical errors
    - Extensible data visualization
    - Slicing and filtering of arrays
    - Powerful expression system
    - Conditional watchpoints
TotalView Remote Display Client

- The Remote Display Client offers users the ability to easily set up and operate a TotalView debug session that is running on another system.
- Provides for a connection that is
  - Easy
  - Fast
  - Secure
- The Remote Display Client is available for:
  - Linux x86
  - Linux x86-64
  - Windows XP
  - Windows Vista
  - Mac OS X Leopard and Snow Leopard
- The Client also provides for submission of jobs to batch queuing systems PBS Pro and LoadLeveler
Batch Debugging with TVScript

- **TVScript**
  - Defines events
    - Breakpoints, memory errors, etc..
  - Actions to take in response to these events
    - Print variables or create memory reports
  - Runs a serial or MPI program towards completion
    - With no user interaction
  - More powerful and flexible than Printf-style debugging
    - Use to prepare and guide interactive debugging
    - Use whenever jobs need to be submitted into a managed environment
    - Can be used to automate test/verify environments

Here, for example, is how tvscript is invoked on a program:
```
    tvscript
    -create_actionpoint "method1=>display_backtrace"
    -show_arguments
    -create_actionpoint "method2#37=>display_backtrace"
    -show_locals -level 1
    -display_specifiers "nowshow_pid.noshow_tid"
    -maxruntime "00:00:30"
    filterapp -a 20
```
You can also execute MPI programs using tvscript. Here is a small example:
```
    tvscript -mpi "Open MP" -tasks 4
    -create_actionpoint
        "hello.c#14=>display_backtrace"
    ~/tests/MPI_hello
```
MemoryScape

Simple to use, intuitive memory debugging

- What is MemoryScape?
  - Streamlined
  - Lightweight
  - Intuitive
  - Collaborative
  - Memory Debugging

- Features
  - Shows
    - Memory errors
    - Memory status
    - Memory leaks
    - Buffer overflows
  - MPI memory debugging
  - Remote memory debugging

- Technical Advantages
  - Low overhead
  - No Instrumentation

- Interface
  - Inductive
  - Collaboration
  - Multi-process
ReplayEngine

- Enhances debugging experience
  - Add-on to TotalView
- Captures execution history
  - Record all external input to program
  - Records internal sources of non-determinism
- Replays execution history
  - Examine any part of the execution history
  - Step as easily back through code as you do forwards
  - Jump to points of interest
- Simple extension to TotalView
  - No recompilation or instrumentation
  - The user just says where they want to go
  - Explore data and state in the past just like a live process
- Supported on Linux x86 and x86-64
- Supports MPI, Pthreads, and OpenMP
TotalView for CUDA

- Characteristics
  - Debugging of application running on the GPU device (not in an emulator)
  - Full visibility of both Linux threads and GPU device threads
    - Device threads shown as part of the parent Unix process
    - Correctly handle all the differences between the CPU and GPU
  - Fully represent the hierarchical memory
    - Display data at any level (registers, local, block, global or host memory)
    - Making it clear where data resides with type qualification
  - Thread and Block Coordinates
    - Built in runtime variables display threads in a warp, block and thread dimensions and indexes
    - Displayed on the interface in the status bar, thread tab and stack frame
  - Device thread control
    - Warps advance synchronously
  - Handles CUDA function inlining
    - Step into or over inlined functions
    - Functions show on stack trace
  - Reports memory access errors
    - CUDA memcheck
  - Multi-Device Support
  - Can be used with MPI
Optimization tool that provides real performance analysis of your running code

Focus attention to the code and the problems that matter and can be solved

What-if analysis from a single sampling

The tool is your mentor – learn as you go, become proficient

Performance regression test tool:
  - because resource contention is a global concern
  - Problems don’t always show up at intuitive places
Cache Optimization Technology

- Analyze binary behavior
  - Collect sparse runtime data
  - Model off-line using math

- ThreadSpotter
  - Application performance analysis for programmers
  - We tell what the problem is, where it is and how to fix it

Makes the performance experts more productive
Enables non-experts to optimize code
Example: Poor parallelism? (LBM)

- Actually, it is “embarrassingly parallel”
- Poor memory usage → super-linear slowdown
The same application optimized (LBM)

- Optimization can be rewarding, but costly...
  - Requires expert knowledge
  - Weeks of wading through performance data
- ThreadSpotter one-click advice: Change one line
Resources

Rogue Wave Software website
• www.roguewave.com

Demystifying debugging whitepaper
• http://www-931.ibm.com/bin/newsletter/tool/landingPage.cgi?lpId=3022

TotalView video tutorials
• http://www.totalviewtech.rs qp1.com/support/videos.html#0

Acumem ThreadSpotter On-line Demo
• https://acumem.webex.com/acumem/ldr.php?AT=pb&SP=MC&rID=19140117&rKey=CD1662E760EA59FE
Visiting SC10?

Visit Rogue Wave at Booths 2431 and 2432 and Acumem at 3749

Contact me if you would like us to schedule a meeting with our senior product and management staff at the event.

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Thank You