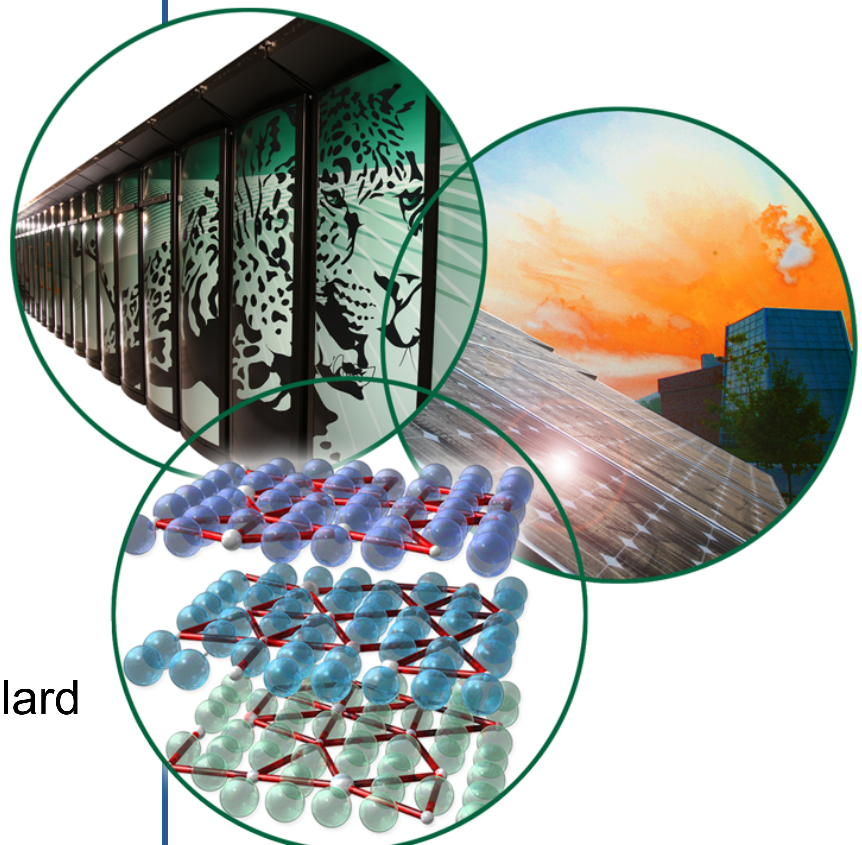
Third Party Tools for Titan



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U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY
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Goals

- Provide OLCF-3 users with high productivity programming languages & compilers.
- Provide a programming environment with tools to support the porting of codes.
- Work with vendors to provide compiler, performance, and debugger capabilities needed to port applications with GPUs :
  - **CAPS enterprise (OpenHMPP Directives)**
  - **The Portland Group (Accelerator Directives)**
  - **Cray (OpenMP for Accelerators)**
  - **NVIDIA**
  - **TU-Dresden (Vampir)**
  - **Allinea (DDT)**
- Joint Standardization Efforts: **OpenACC, OpenMP ARB**

Improve Productivity and Portability

- The Directive based approach provides:
  - Incremental porting/development
  - Fast Prototyping
    - The programmer can quickly produce code that runs in the accelerator
  - Increases Productivity
    - Few code modifications to produce accelerated code
  - Retargetable to different architectures (CPU, GPUs, FPGAs)
  - Tools can assist the user generate the directives, debug them, and do performance analysis
- Leading technologies with accelerator directives:
  - OpenACC directives (Cray, PGI, CAPS, NVIDIA)
  - CAPS OpenHMPP directives
  - PGI accelerator directives

Compilers Available for OLCF-3

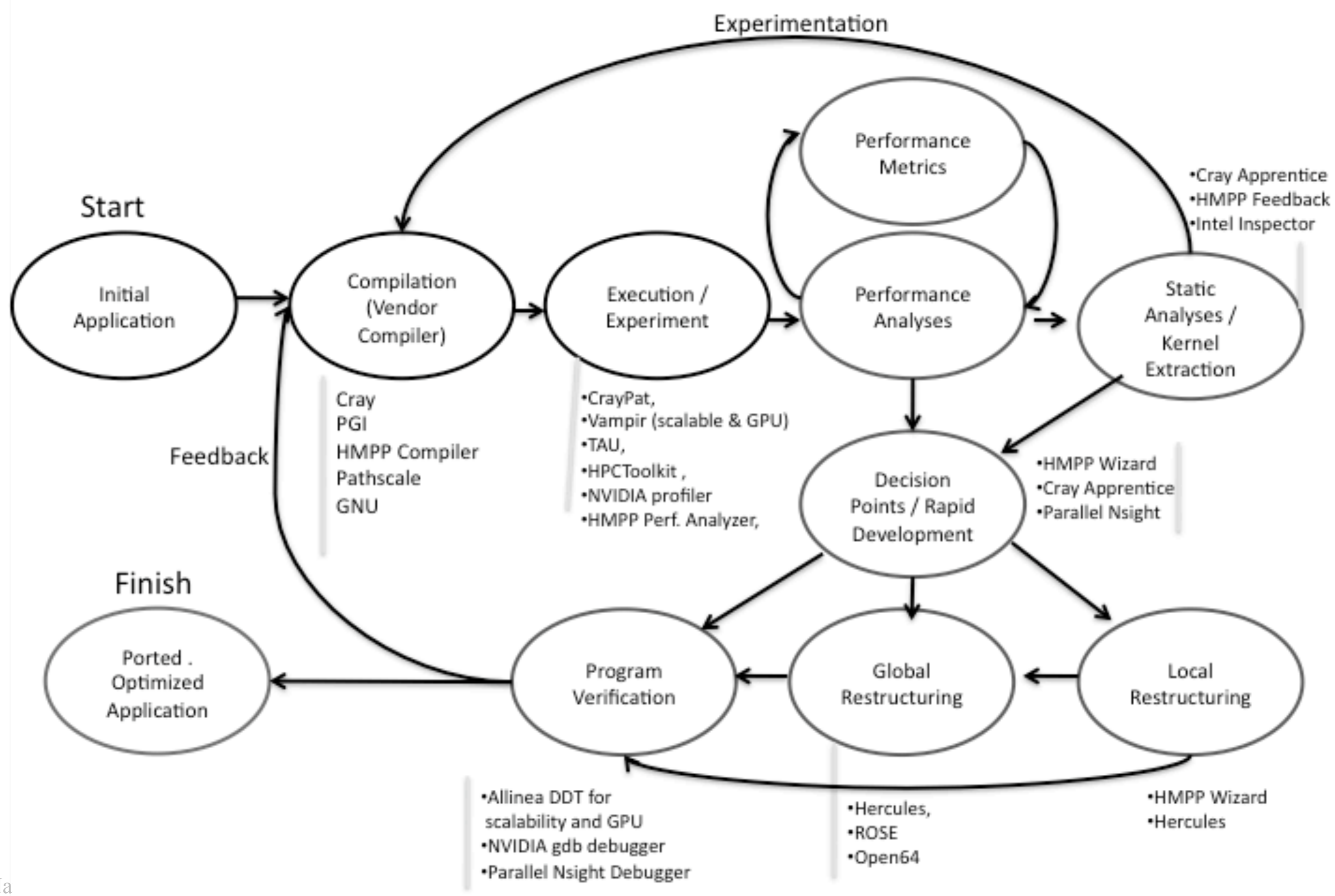
Compiler Vendor	C/C++	Fortran	CUDA C / OpenCL	CUDA Fortran	OpenHMPP	PGI Acc Dir	OpenACC	OpenMP CPU
Cray	X	X					X	X
PGI	X	X	P	X		X		X
CAPS HMPP	X	X			X		X	X
NVIDIA			X					
Pathscale	X	X			P		P	X
Intel	X	X						X
GNU	X	X						X

X = Supported
P = In Progress

• Cray, CAPS, and NVIDIA are directly involved with the OLCF-3 Effort

Current Work

- We are currently working with Vendors to provide a set of tools that target the application needs for OLCF-3
- We are also building a tool environment to support the applications:

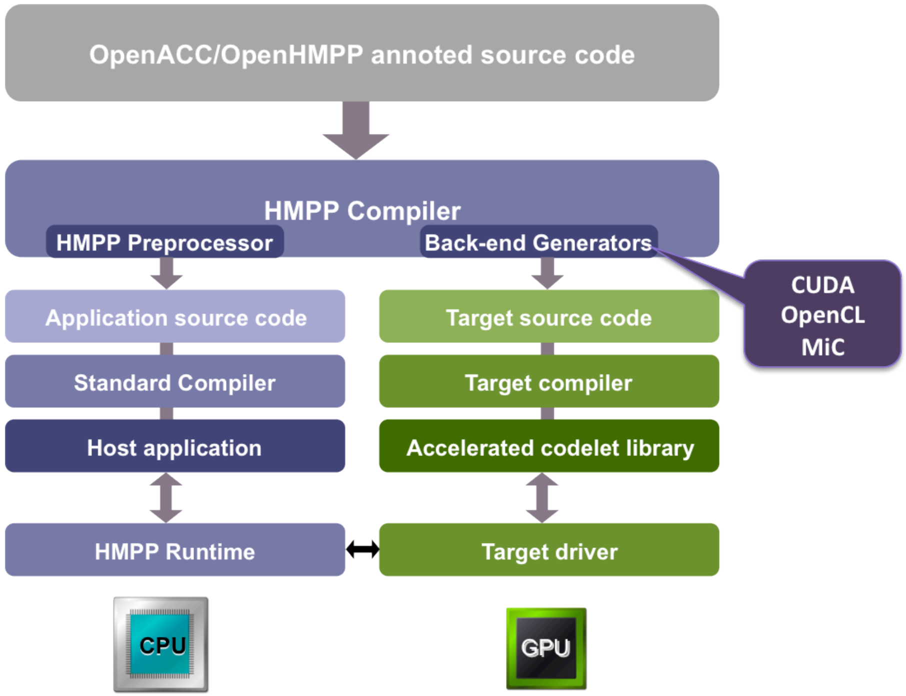


Programming Models

- System supports: C/C++/Fortran, OpenMP, MPI, SHMEM
- GPU accelerator directives: OpenACC and OpenHMPP directives
- We identified features needed for programmability, performance improvements or bugs.
  - C++ support [Feature]
  - Fortran module support [Feature]
  - Inlining support [Feature]
  - Need to allocate data directly in the GPU [Performance]
  - 3D scheduling support for thread blocks [Performance]
  - Support for libraries [Feature]
  - Codelet functions [Feature]
  - Worksharing between devices in nodes. [Feature]

HMPP Overview

- C/Fortran OpenHMPP and OpenACC directive-based programming model (API-based for C++)
  - Offload functions and regions onto accelerators
  - Manage CPU-GPU data movements
  - Finely tune loop optimizations and use of hardware specific features
  - Complementary to OpenMP and MPI
- A source-to-source HMPP compiler
  - Generates CUDA/OpenCL/MiC kernels
  - Works with standard compilers
- A runtime library
  - Dispatch computations on available GPUs
  - Scale to multi-GPU systems



HMPP Enhanced Features: Driven by OLCF Application Needs

- MADNESS:
  - API for C++ applications
- LAMMPS:
  - Multi-GPU and CPU data distribution
- LSMS:
  - Seamless integration of accelerated libraries

HMPP for C++ Applications

- Runtime API close to OpenCL with one directive to let HMPP generate the CUDA version of a function

```
template<typename T>
void add_vector(int n, T * y, T * a, T * b)
{
  for(int i = 0 ; i < n ; i++)
      y[i] = a[i] + b[i];
}

// Instantiate the add_vector<float> template and
// associate it to the codelet "add_vector_float"
#pragma hmppcg entrypoint as add_vector_float, target=CUDA
template void add_vector<float>(int n, float *y,
                                float *a, float *b);
```

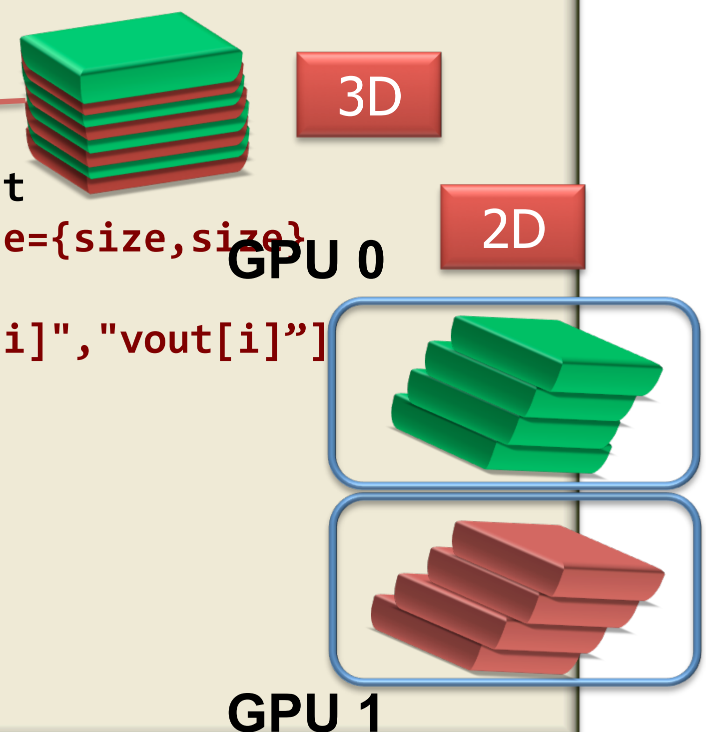
- Templates not supported by OpenACC
- MADNESS – heavily dependent on templates

HMPP Data Distribution

- Directives for C and Fortran
  - Define a multi-GPU data distribution scheme and let HMPP execute over multiple devices

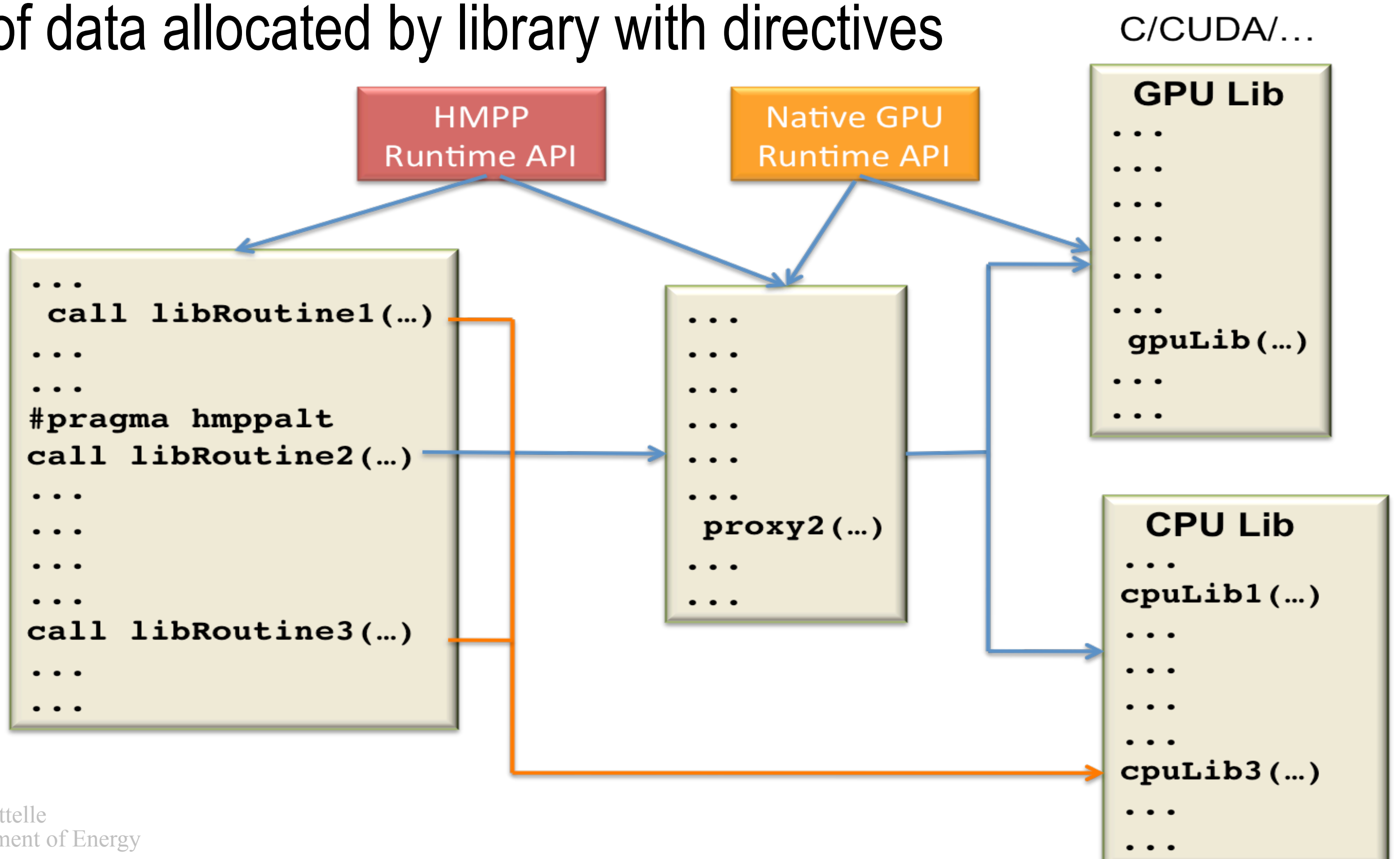
```
float vin1[NB][SIZE][SIZE], vin2[NB][SIZE][SIZE], vout[NB][SIZE][SIZE];
. . .

#pragma hmpp parallel, device="i%2"
  for( i=0;i<NB;i++) {
   //Allocate the mirrors for vin1, vin2 and vout
#pragma hmpp allocate, data["vin1[i]”, ...], size={size,size}
    //Transfer data to the GPU from the mirrors
#pragma hmpp advancedload, data["vin1[i]","vin2[i]","vout[i]”]
    ...
#pragma hmpp sgemm callsite
    sgemm( vin1[i], vin2[i], vout[i] );
    ...
//Get back the result
#pragma hmpp delegatedstore, data["vout[i]"]
   }
```



HMPP Accelerated Library Integration

- Use accelerated libraries as an alternative to the original library
  - Keep one single source code with CPU and GPU libraries
  - Uses hmppalt directives with a proxy mechanism
- Compatible with CUBLAS, MAGMA, CULA libraries
- Access of data allocated by library with directives



LSMS case study

- Already existing GPU version using cuBLAS and CULA libraries

```
do iblk=nblk,2,-1
    ...
    call cula_device_zgetrf(...)
    call cula_device_zgetrs(...)
    call cublas_zgemm(...)
    call cublas_zgemm(...)
enddo
call cublas_zgemm(...)
call cublas_get_matrix(...)
```

```
!$hmppalt myproxy declare, name="zgemm", fallback=true
SUBROUTINE lsmszgemm(error,transa,...)
...
END SUBROUTINE lsmszgemm

!$hmppalt lsms declare, name="zgetrf", fallback=true
SUBROUTINE lsmszgetrf(error, m, n, a, lda, ipiv,
info)
...
END SUBROUTINE lsmszgetrf
...
!$hmpp advancedload
do iblk=nblk,2,-1
!$hmppalt myproxy
call zgetrf(...)
…
!$hmppalt myproxy
call zgemm(...)
!$hmppalt myproxy
call zgemm(...)
enddo
```

Declare proxy interfaces

Call HMPP alternative library while keep original call in place

Vampir Toolset

- **VampirTrace**
  - Application instrumentation
  - Pre-run phase
  - Via compiler wrapper, library wrapper and/or third-party software
  - Measurement
  - Event collection (functions calls, MPI, OpenMP, performance counter, memory usage, I/O, GPU)
  - Timer synchronization
  - Filtering and grouping of events

- **Vampir (Client and Server)**
  - Trace visualization software
  - Alternative and supplement to automatic analysis
  - Show dynamic run-time behavior graphically
  - Provide statistics and performance metrics
  - Interactive browsing, zooming, selecting capabilities

Vampir Performance Analysis Tools

- Custom improvements for the OLCF-3 system
- Focused on three main areas
  - Scaling the Vampir tools to higher processor counts
  - Integrating GPU support for a comprehensive analysis of heterogeneous systems
  - Additional usability enhancements

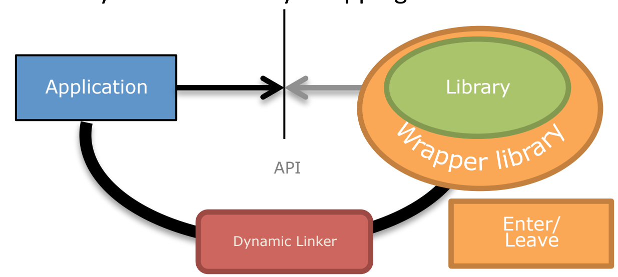
Vampir toolset challenges

- Support for GPU tracing
- Scaling up to a Titan-sized HPC-system
- Overcome I/O challenges related to the huge amount of data generated by traces as well as the number of tracing streams
- General enhancements in terms of usability and analysis possibilities

Vampir GPU support for Titan

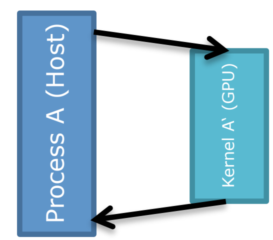
- Successive CUDA support based on latest CUDA releases
- How CUDA fits into Vampir's design
  - accelerator threads treated like OMP threads
  - CUDA memcpy treated like MPI communication
- Tracing of multiple CUDA kernels in one executable
- Tracing of asynchronous GPU events
- Tracing of performance counters on GPUs

Currently done via library wrapping

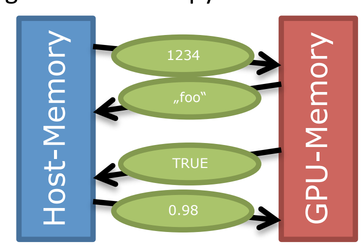


Reuse of known metrics:

Thread = Kernel



Message = cudaMemCpy



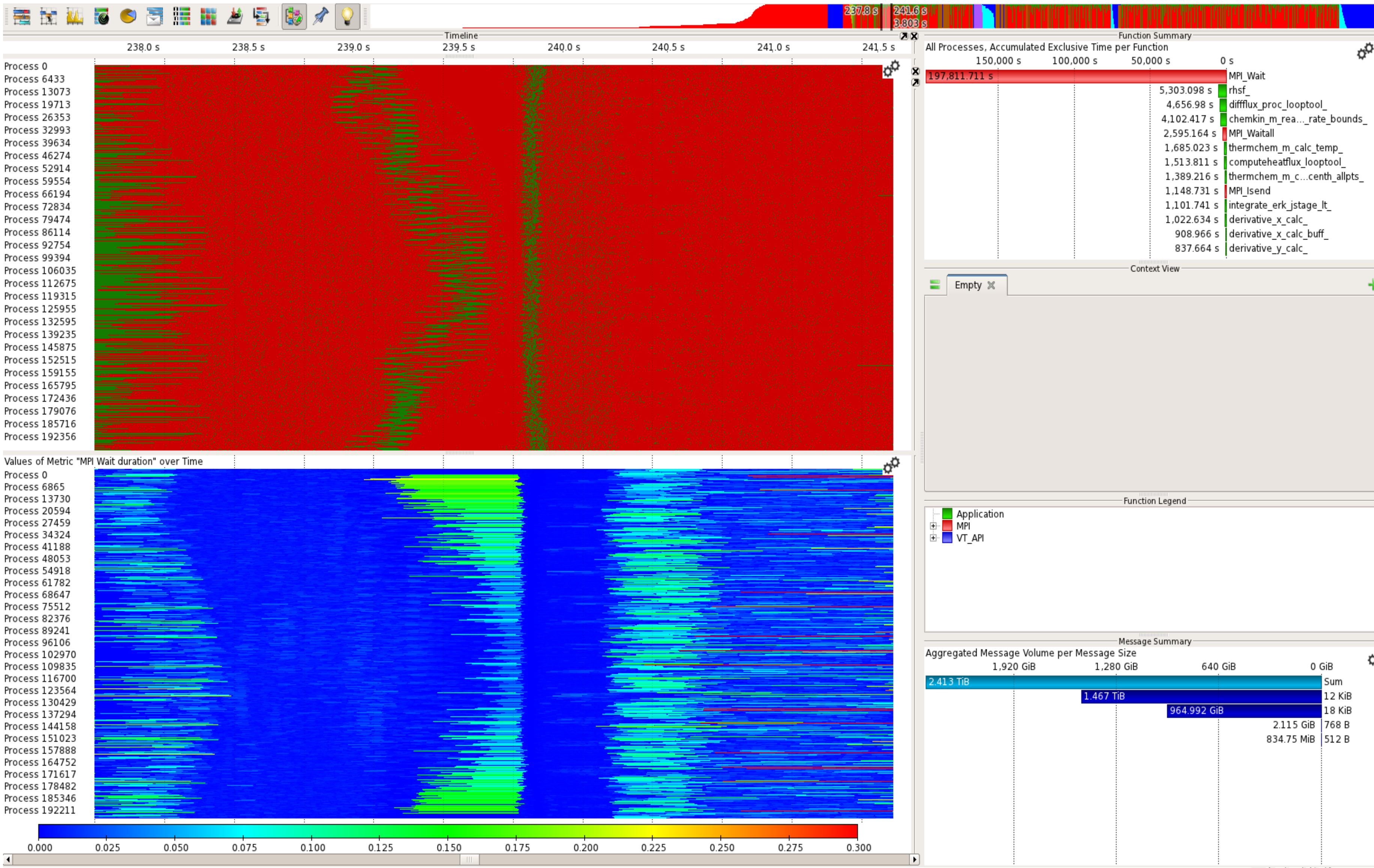
Vampir Scalability Improvements

- Parallelization of VampirTrace tools: otfmerge, vtfilter, otfprofile
  - enable the processing of traces with >10k streams!!
- Enhanced output of otfprofile
  - Global message statistics
  - Time spent in MPI
  - Process clustering information
- Improved MPI behavior of VampirServer
  - Analyze traces with >10k analysis processes
  - Allows to analyze traces on the entire Titan system
- New displays
  - Performance radar (performance counter for all processes over time)
  - Highlight performance bottlenecks (related to counters)

I/O Challenge

- Online trace file compression (reduce i/o load)
  - Find pattern and record only one (aka rewind)
  - Find pattern irregularities: use marker to highlight pattern irregularities
- Visualization of those compressed traces via multiplexing the recorded pattern (only in the display, not in memory) to show the trace as a whole
- Use IOFSL to aggregate large number of streams in a small number of files (instead of saving each stream in one file) to reduce the load for the Lustre meta data server

S3D on Jaguar (200k+ cores)

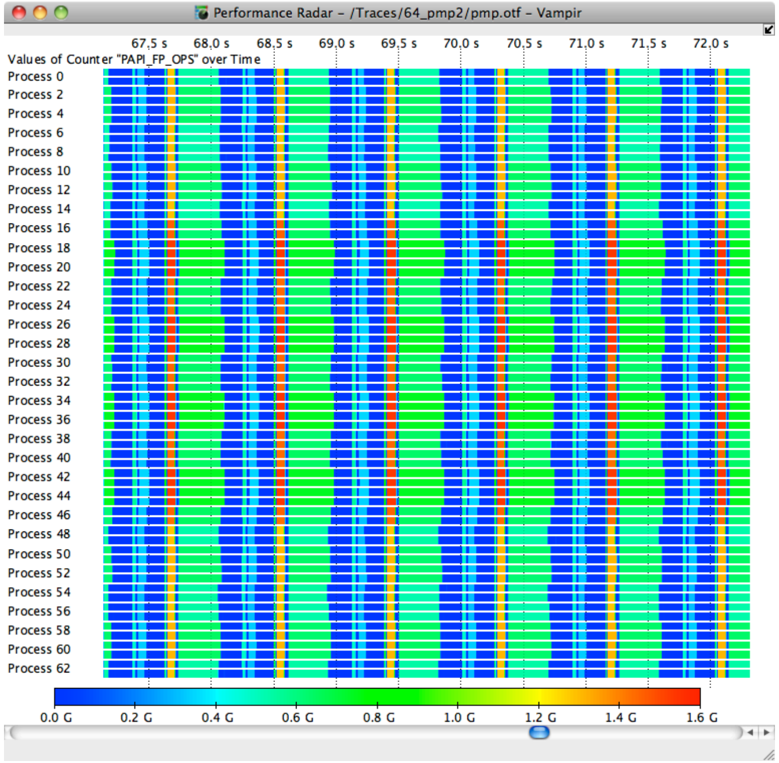


Vampir Usability/Analysis Enhancements

- Vampir clients for all major OS platforms (Linux, Mac, Win)
- Automatic generation of filter files (based on previous runs) to trace only performance relevant parts
- Performance Radar
  - Derived counters
  - Highlighting of function anomalies based on user defined thresholds
- Enhanced filtering capabilities
  - functions, functions groups, processes inside of Vampir
- Compare View
  - Compare multiple traces directly, while showing them in one display

Vampir Usability/Analysis Enhancements

Performance Radar



Compare View

 Managed by UT-Battelle
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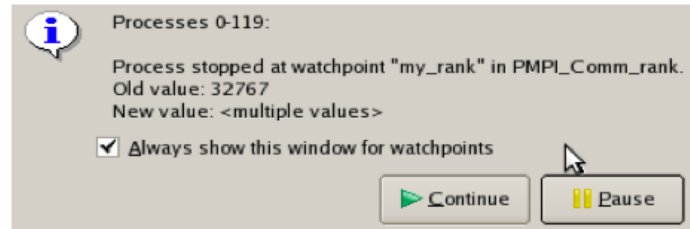
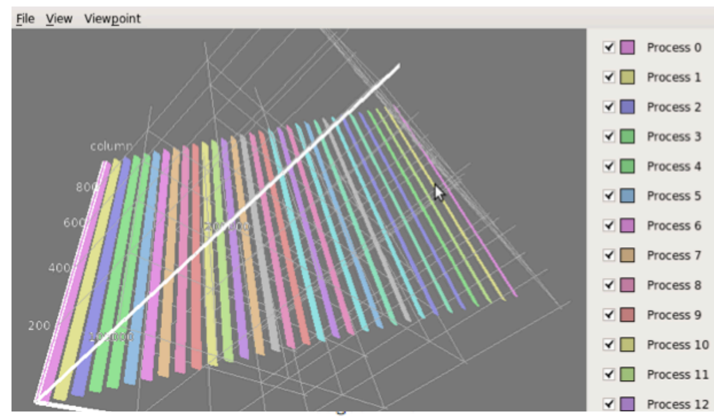
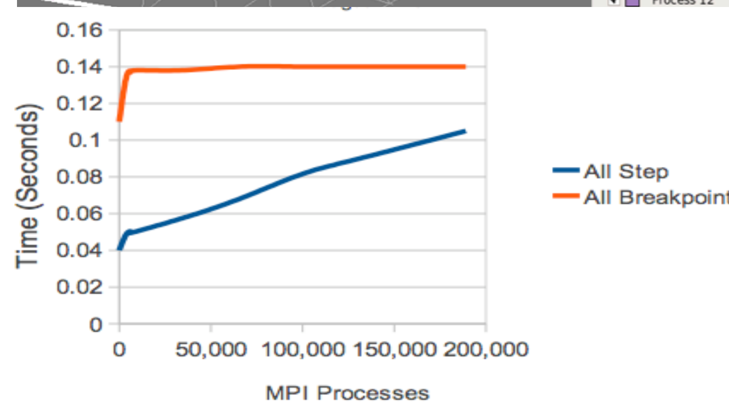
Allinea DDT Debugger

- Work with Allinea to improve the scalability of the DDT debugger
- Data Analysis
  - Parallel Watchpoints
  - Addition of “sparklines”
  - Scalable data analysis
  - Scalable breakpoints, stepping and program stack queries
- Major GPU enhancements







DDT Integration with Cray PE

- Support for Abnormal Process Termination (APT), allows to attach DDT to aborted process and review stack

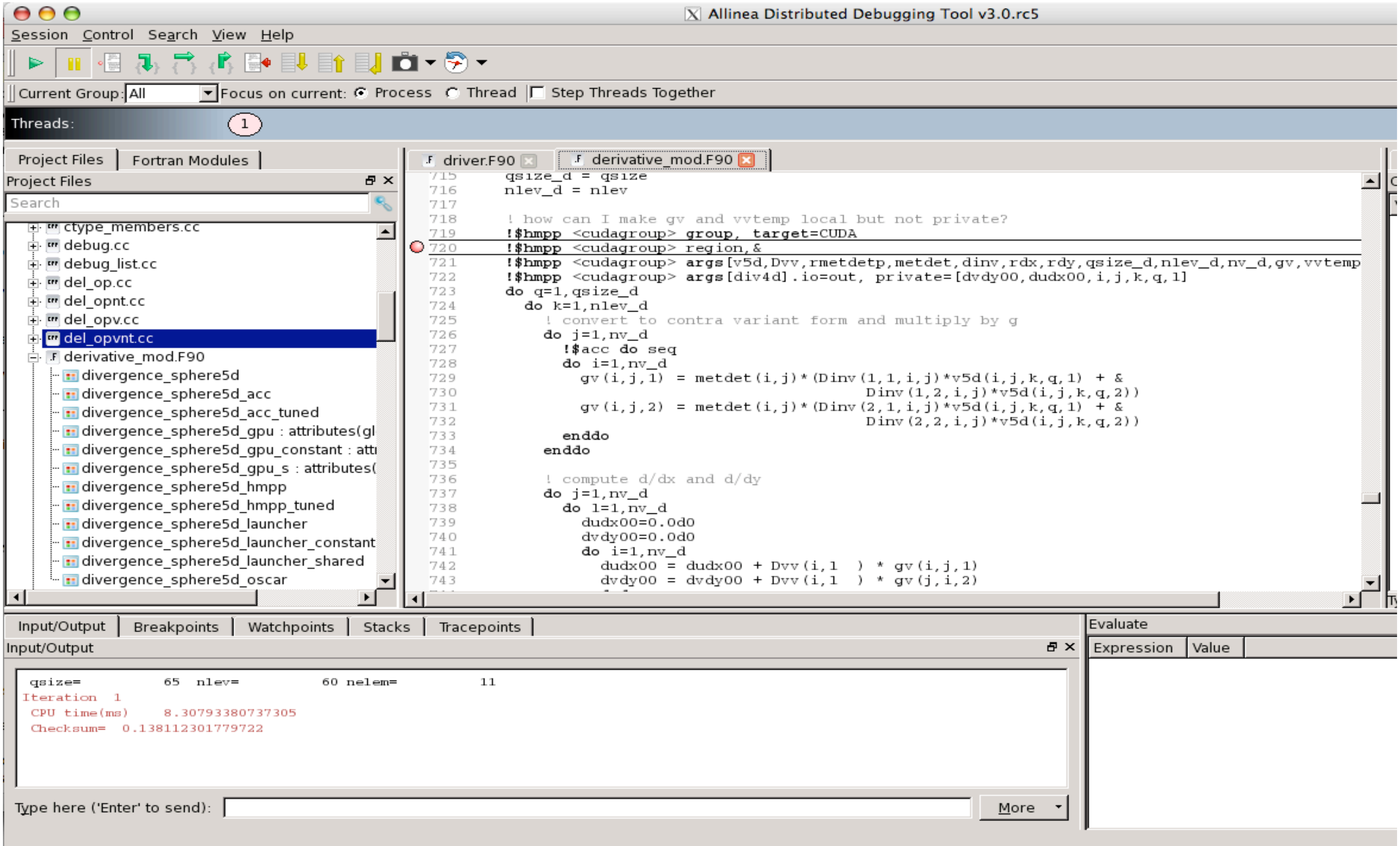
```
Application 1110443 is crashing. ATP analysis proceeding...

Stack walkback for Rank 23 starting:
  _start@start.S:113
  __libc_start_main@libc-start.c:220
  main@atploop.c:48
  __kill@0x4b5be7
Stack walkback for Rank 23 done
Process died with signal 11: 'Segmentation fault'
View application merged backtrace tree file 'atpMergedBT.dot' with
'statview'
You may need to 'module load stat'.

atpFrontend: Waiting 5 minutes for debugger to attach...
```

- Multiple core file support using xt_setup_core_handler()
- Open MPI (Cray XK/alps) version support

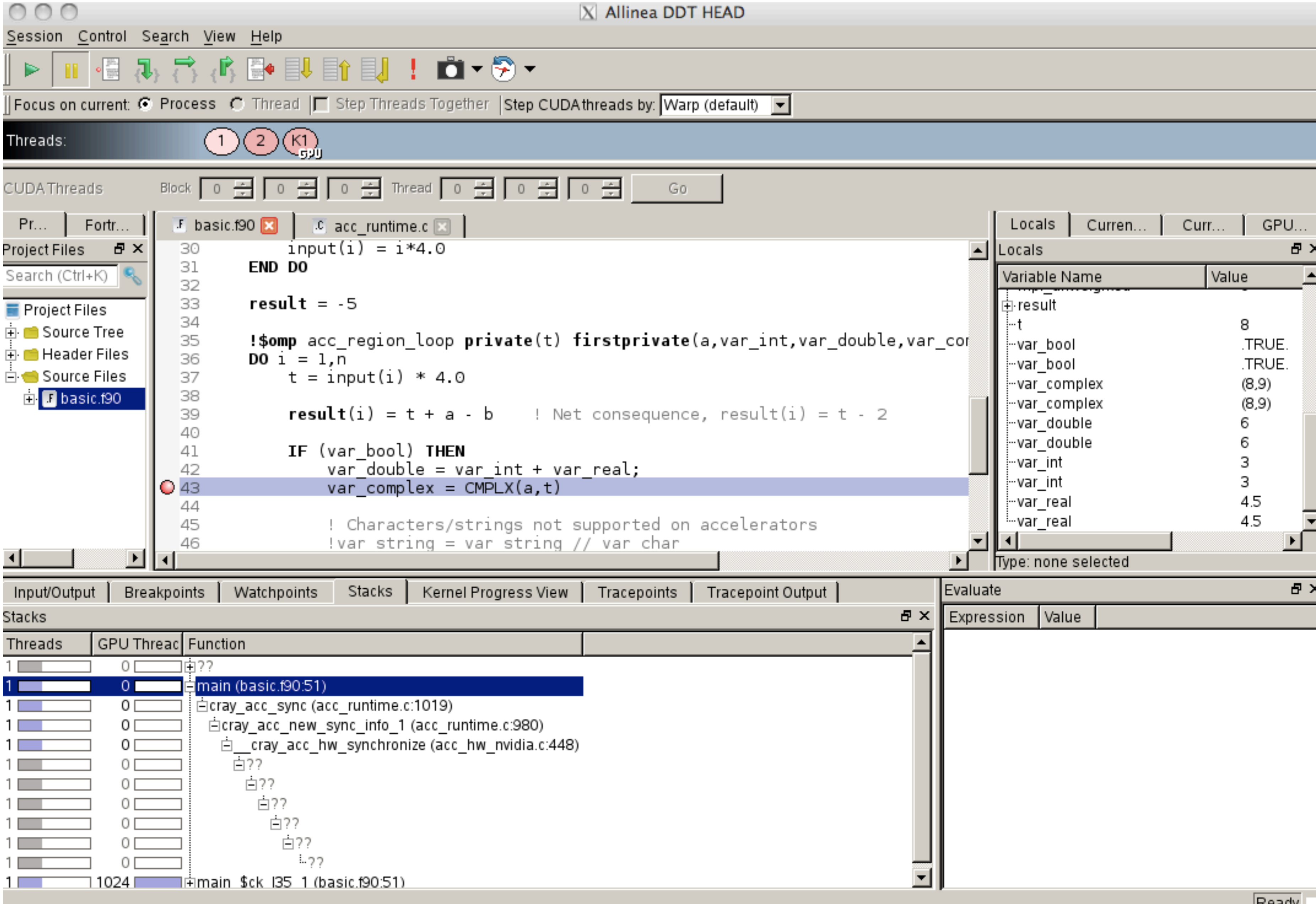
DDT GPU Support

- Cray compiler support
  - Stepping into OpenACC regions
  - Setting breakpoints within OpenACC regions
- Support for HMPP directives
  - stepping into HMPP codelets
- Multiwarp stepping in CUDA codes
- CUDA memory debugging capabilities
  - Identify memory leaks on the device
  - Visual display of memory allocated on host and device

DDT Debugging with HMPP directives

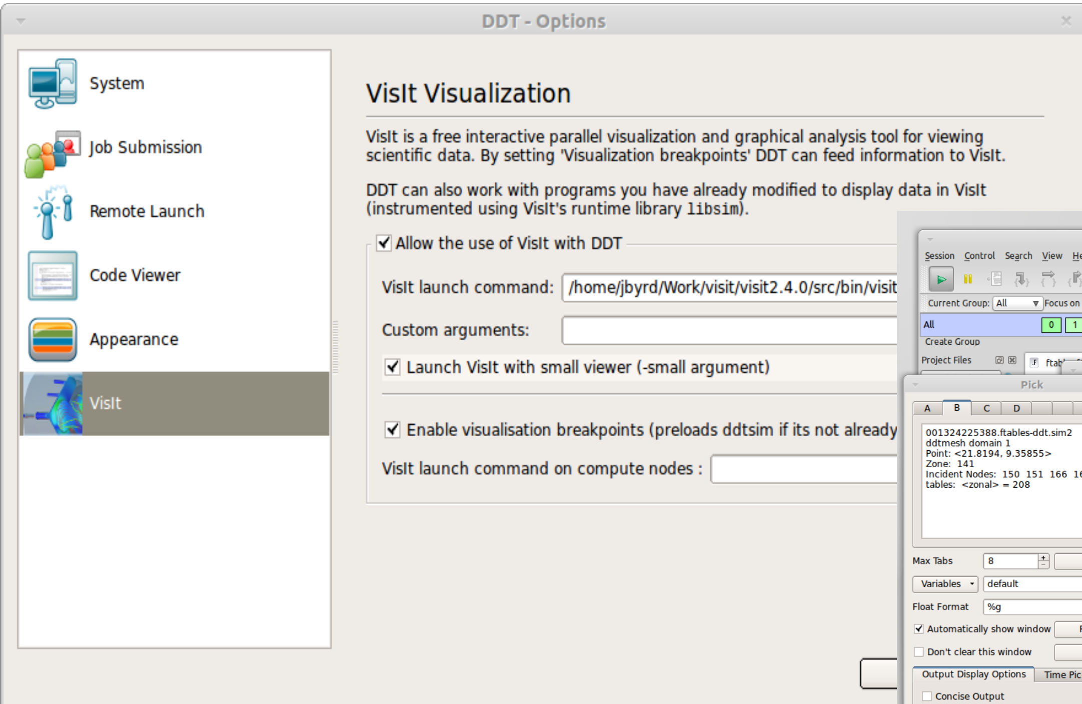


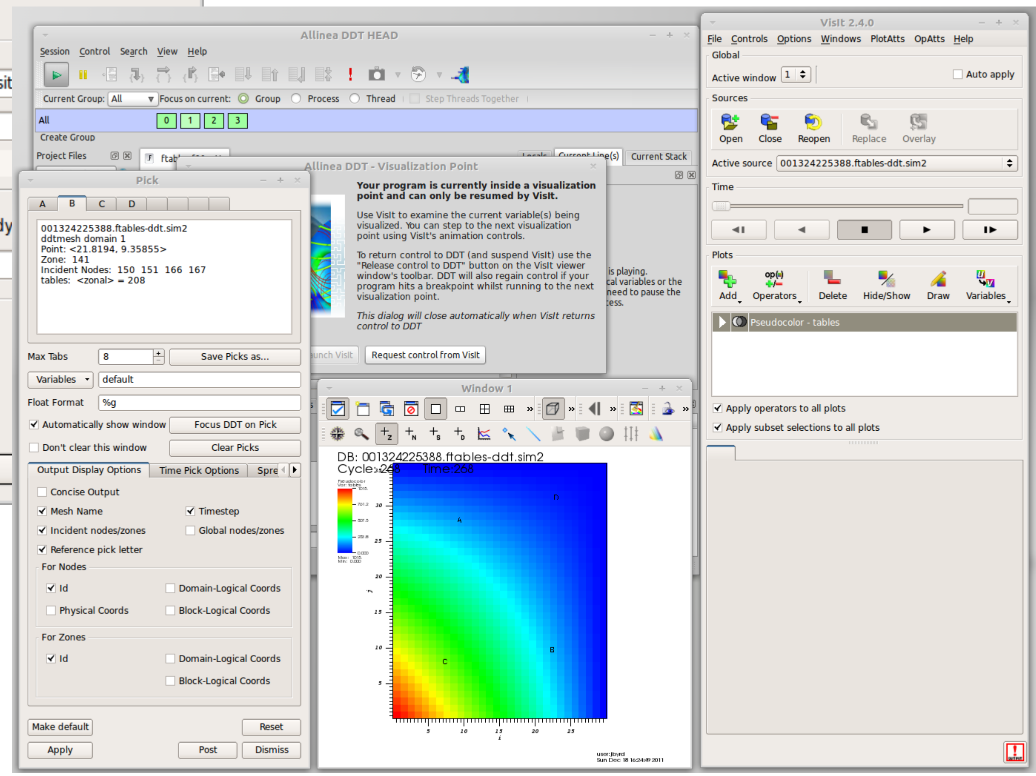
DDT and OpenACC Directives



DDT and VisIT

- Integration with VisIT (Available with VisIT 2.5 summer 2012)
  – Coupling advanced application generated data visualization capabilities with scalable debugging





Thank you for your attention!

- Questions and comments are most welcome