Intel® Tuning for Juwels and Jureca

Dr. Heinrich Bockhorst

FZJ 2025, May 15th

intel®

Agenda

- oneAPI Initiative
- Intel® Compiler
- Application Performance Snapshot (APS)
- VTune Profiler
- Advisor
- MKL and MPI

oneAPI Industry Initiative

Break the Chains of Proprietary Lock-in

Freedom to Make Your Best Choice

- One programming model for multiple architectures and vendors
- Cross-architecture code reuse for freedom from vendor lock-in

Realize all the Hardware Value

- Performance across CPU, GPUs, FPGAs, and other accelerators
- Expose and exploit cutting-edge features of the latest hardware

Develop & Deploy Software with Peace of Mind

- Open industry standards provide a safe, clear path to the future
- Compatible with existing languages and programming models including C, C++ with SYCL, Python, OpenMP, Fortran, and MPI
- Powerful libraries for acceleration of domain-specific functions

oneAPI

The productive, smart path to freedom for accelerated computing from the economic and technical burdens of proprietary programming models

KHRONOS GROUP SYCL

Intel® oneAPI DPC++/C++ Compiler

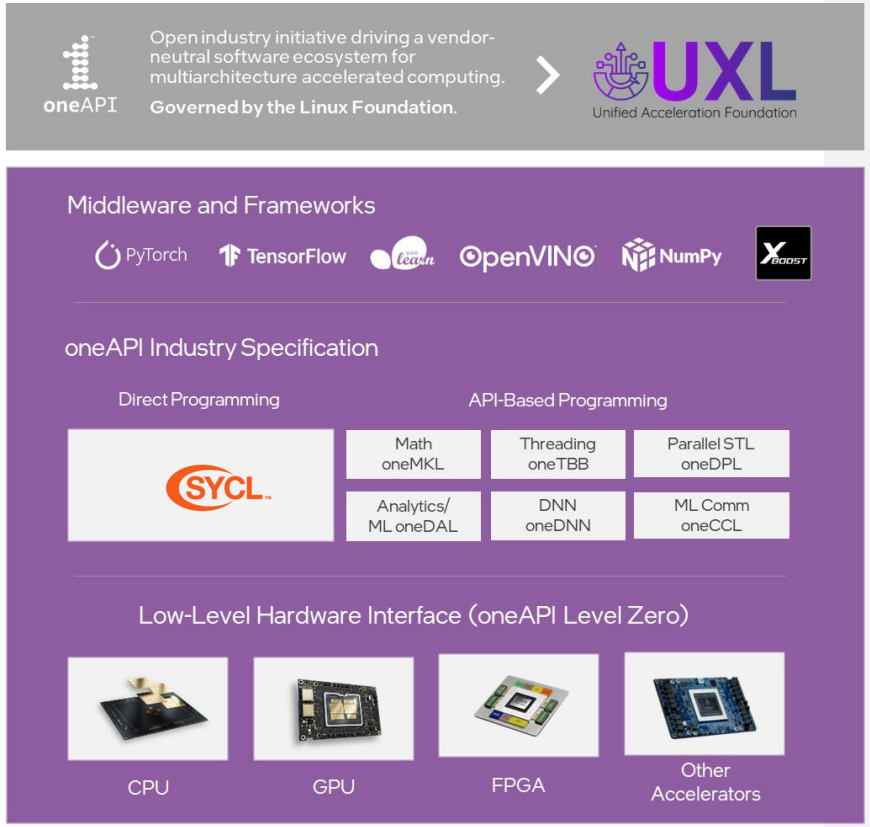
Conformant with SYCL 2020 Specification

Unified Shared Memory Parallel Reductions, Work Group Algorithms, Class Template Argument Deductions, Simplification of Accessors, Expanded Interoperability, and more …

An Industry First:
SYCL 2020 Conformance on CPU and GPU

Intel is proud to contribute to a revolution anchored in SYCL:

An open ecosystem of
- software developers
- hardware vendors
- compilers and development tools
- APIs and specifications



Intel® oneAPI DPC++/C++ Compiler:
with SYCL towards Open Multiarchitecture Computing

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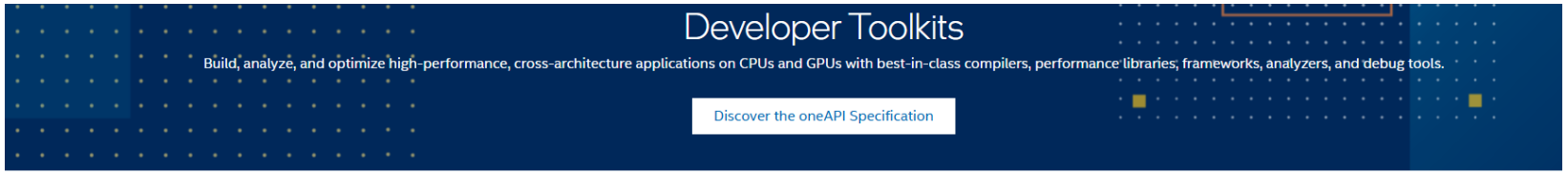
Toolkits for Developer: free download



Select Your Toolkit

Download what you need for any project.

Intel® oneAPI Base Toolkit

Develop performant, data-centric applications across Intel® CPUs and GPUs with this foundational toolset.

General Compute

- Intel® oneAPI DPC++/C++ Compiler
- Intel® DPC++ Compatibility Tool
- Intel® Distribution for GDB*
- Intel® oneAPI DPC++ Library (oneDPL)
- Intel® oneAPI Threading Building Blocks (oneTBB)
- Intel® oneAPI Math Kernel Library (oneMKL)
- Intel® oneAPI Deep Neural Networks Library (oneDNN)
- Intel® oneAPI Data Analytics Library (oneDAL)
- Intel® oneAPI Collective Communications Library (oneCCL)
- Intel® Integrated Performance Primitives (Intel® IPP)
- Intel® Cryptography Primitives Library
- Intel® Advisor
- Intel® VTune™ Profiler

Learn More

Download

Intel® oneAPI HPC Toolkit

Build, analyze, and scale HPC applications across shared and distributed memory computing systems.

High-Performance Computing

- Intel oneAPI DPC++/C++ Compiler
- Intel® Fortran Compiler
- Intel DPC++ Compatibility Tool
- Intel Distribution for GDB
- Intel oneAPI Threading Building Blocks (oneTBB)
- Intel oneAPI DPC++ Library (oneDPL)
- Intel® MPI Library
- Intel oneAPI Math Kernel Library (oneMKL)
- Intel oneAPI Deep Neural Networks Library (oneDNN)
- Intel oneAPI Data Analytics Library (oneDAL)
- Intel oneAPI Collective Communications Library (oneCCL)
- Intel® SHMEM
- Intel Integrated Performance Primitives (Intel IPP)
- Intel Cryptography Primitives Library
- Intel Advisor
- Intel VTune Profiler

Learn More

Download

AI Frameworks & Tools

Accelerate end-to-end data science and machine learning pipelines using Python* tools and frameworks.

End-to-End AI and Machine Learning Acceleration

- Python 3.9
- Intel® Extension for PyTorch* (CPU)
- Intel Extension for PyTorch (GPU)
- Intel® Extension for TensorFlow* (CPU)
- Intel Extension for TensorFlow (GPU)
- Intel® Optimization for XGBoost*
- Intel® Extension for Scikit-learn*
- Modin*
- Intel® Neural Compressor

Learn More

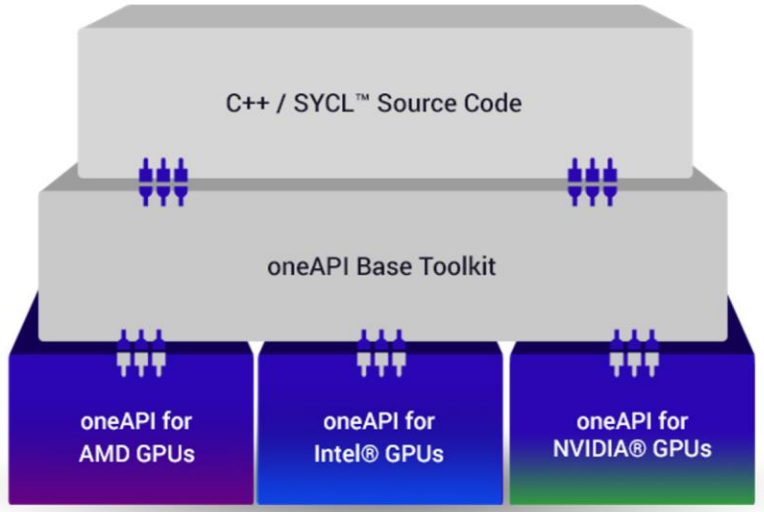
Download

oneAPI for NVIDIA & AMD GPUs

- Free download of binary plugins to Intel® oneAPI DPC++/C++ Compiler:
  - Nvidia GPU
  - AMD GPU
- No need to build from source!
- Plug-ins updated quarterly in sync with SYCL 2020 conformance & performance

Priority Support

- Available through Intel, Codeplay & our channel
- Requires Intel Priority Support for Intel oneAPI DPC++/C++ Compiler
- Intel takes first call, Codeplay delivers backend support
- Codeplay provides access to older plug-in versions

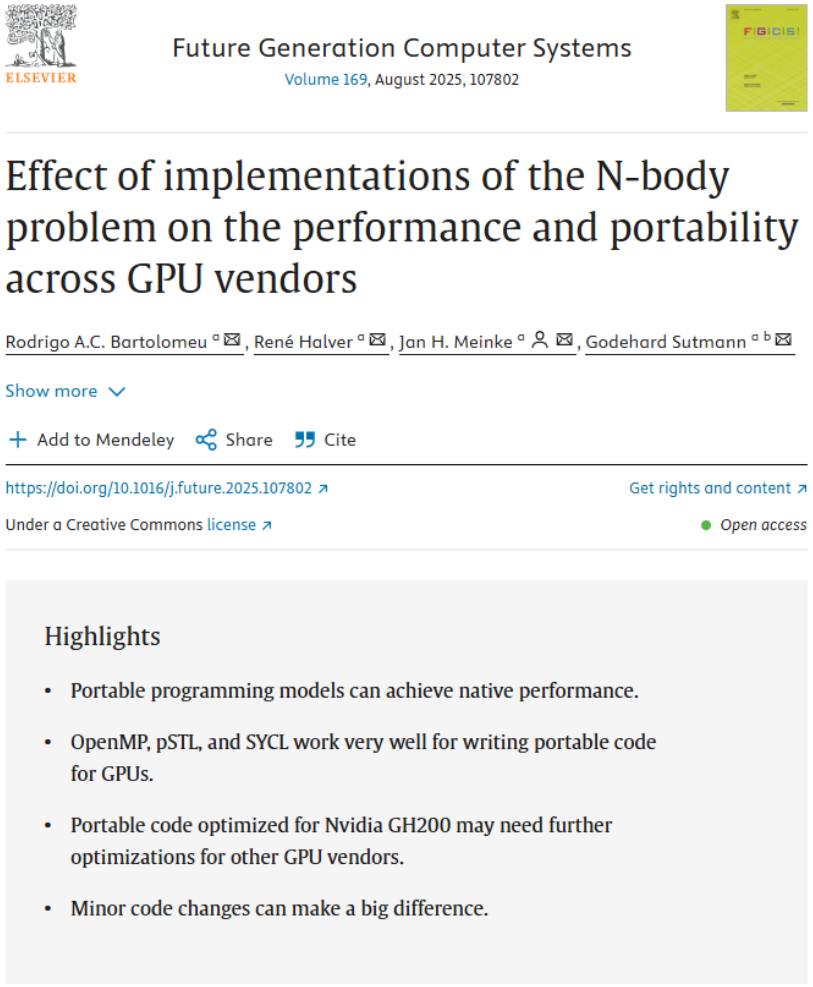


Nvidia GPU plug-in

AMD GPU plug-in

Codeplay blog

Paper on Performance Portability by Jülich Scientists



ELSEVIER

Future Generation Computer Systems
Volume 169, August 2025, 107802

Effect of implementations of the N-body problem on the performance and portability across GPU vendors

Rodrigo A.C. Bartolomeu [a] ✉, René Halver [a] ✉, Jan H. Meinke [a] ✉, Godehard Sutmann [a b] ✉

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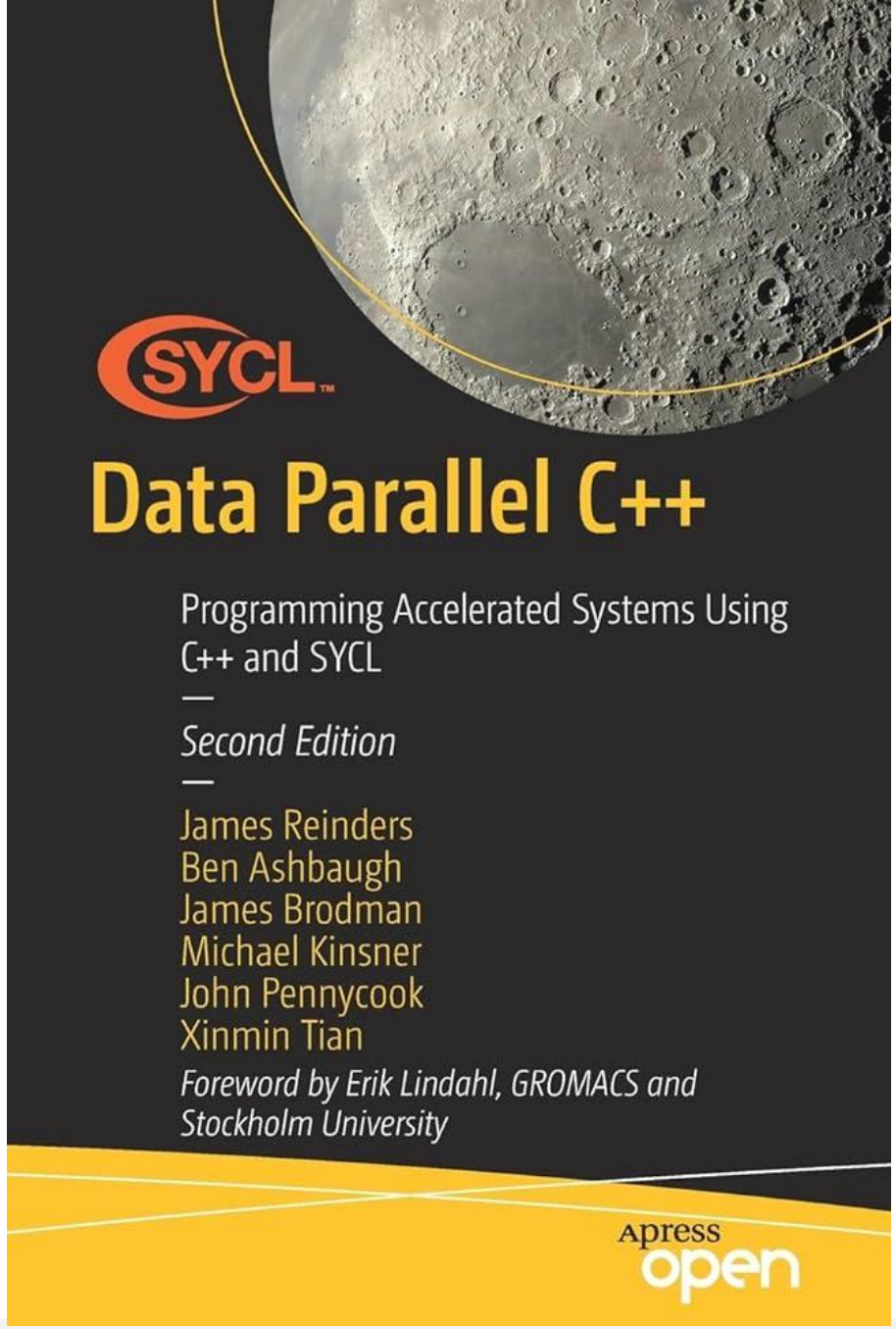
Highlights

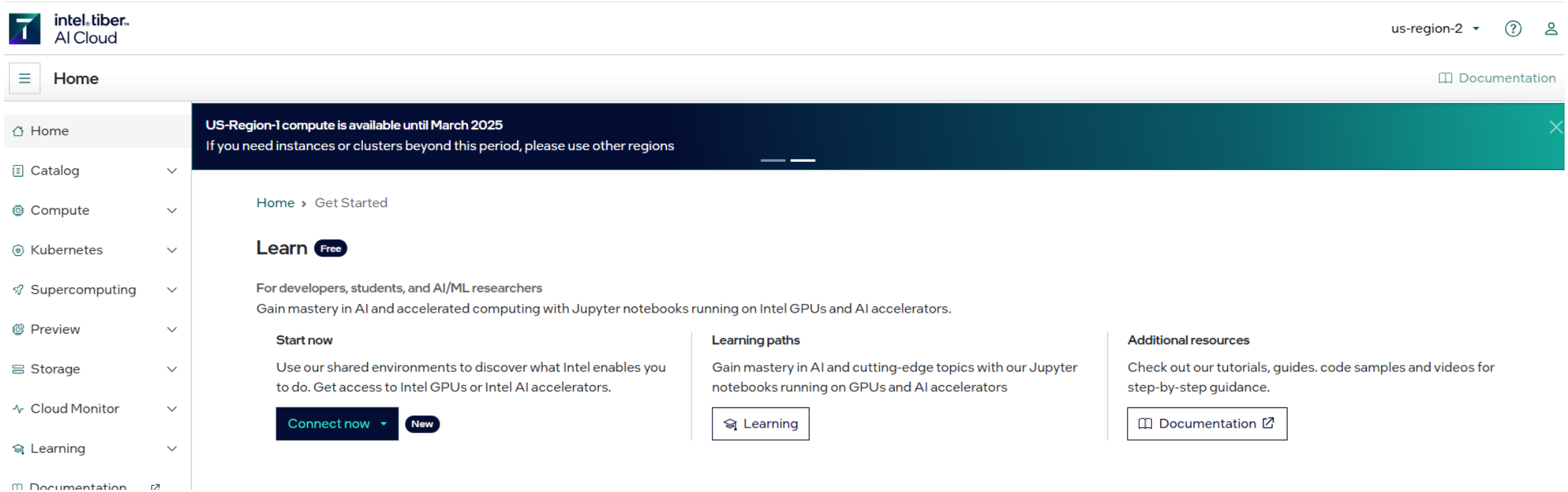
- Portable programming models can achieve native performance.
- OpenMP, pSTL, and SYCL work very well for writing portable code for GPUs.
- Portable code optimized for Nvidia GH200 may need further optimizations for other GPU vendors.
- Minor code changes can make a big difference.

Learn more about SYCL

- New SYCL book covering Khronos Group SYCL 2020 specification and more
- Heterogeneous programming using C++ with SYCL for CPU, GPU, FPGA, and other accelerators
- From foundations to advanced concepts
- Download a free copy https://link.springer.com/book/10.1007/978-1-4842-9691-2



Intel® Tiber™ Cloud – cloud.intel.com



Intel® Compilers

Intel® Compilers

Intel Compiler	Target	OpenMP Support	OpenMP Offload Support	Included in oneAPI Toolkit
Intel® C++ Compiler Classic, IL0 *icc/icpc/icl*	CPU	Yes	No	Removed 2025
Intel® Fortran Compiler Classic, IL0 *ifort*	CPU	Yes	No	Removed 2025
Intel® Fortran Compiler, LLVM *ifx*	CPU, GPU	Yes	Yes	HPC
Intel® oneAPI DPC++/C++ Compiler, LLVM *icx/icpx*	CPU GPU*	Yes	Yes	Base/HPC

Compiler Binary Compatible and Linkable!

tinyurl.com/oneapi-standalone-components

Common optimization options

	Linux* icx (icc)
Disable optimization	-O0
Optimize for speed (no code size increase)	-O1
Optimize for speed (default)	-O2
High-level loop optimization	-O3
Create symbols for debugging	-g
Multi-file inter-procedural optimization	-ipo
Profile guided optimization (multi-step build)	-fprofile-generate (-prof-gen) -fprofile-use (-prof-use)
Optimize for speed across the entire program ("prototype switch")	-fast same as "-ipo -O3 -static -fp-model fast" (-ipo -O3 -no-prec-div –static -fp-model fast=2 -xHost)
OpenMP support	-fiopenmp (-qopenmp)

IFX: Driving a New Era in Accelerated Computing

IFX: ALL that you like in IFORT *PLUS*

- OpenMP* 5.x and 6.0 Standards, offload to Intel GPUs from Fortran
  An open, portable Standard maintains your investment
  Best in class OpenMP features and support
- Fortran 2018 DO CONCURRENT supports automatic offload to Intel GPUs

Protecting your Fortran Investment

Same Fortran parser/analyzer you know and love from IFORT

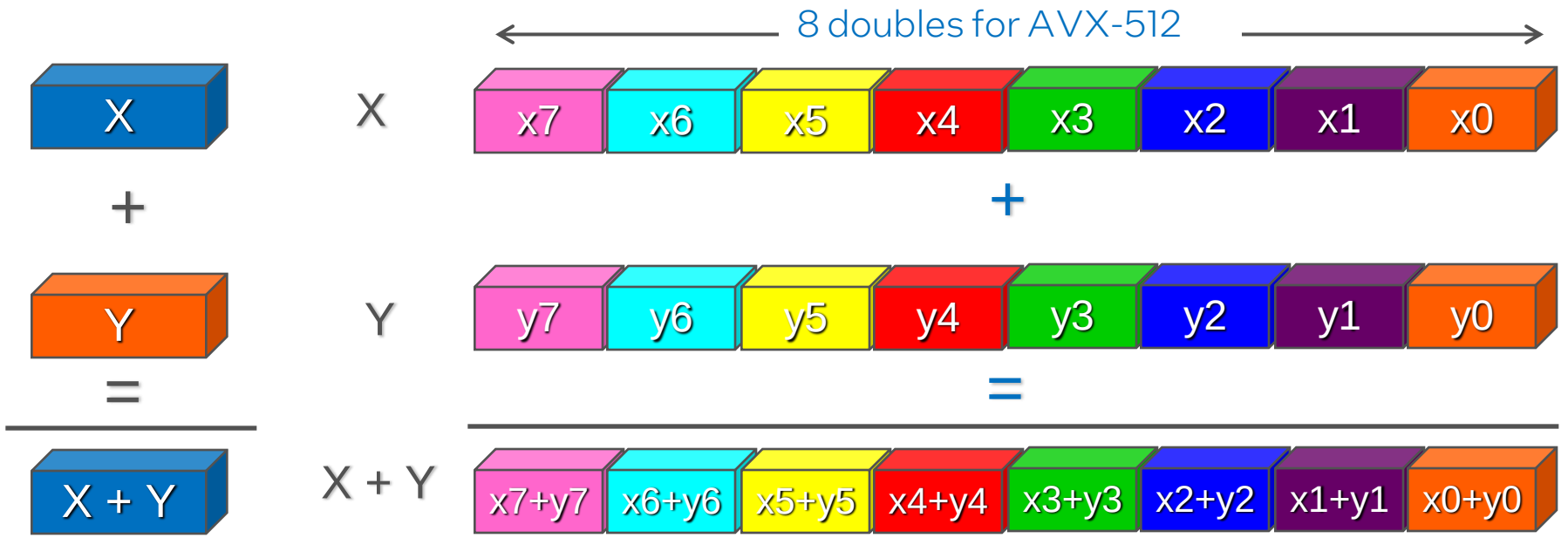
- Supports legacy DEC extensions, ***all F2018,*** ifort directives and features
- The majority of IFORT compiler directives and options you have used for years. And Microsoft Visual Studio* integration for Windows*

Binary compatible, mix and match ifx and ifort

SIMD: Single Instruction, Multiple Data

```
for (i=0; i<n; i++) z[i] = x[i] + y[i];
```

- Scalar mode
  - one instruction produces one result
  - E.g. vaddss, (vaddsd)
- Vector (SIMD) mode
  - one instruction can produce multiple results
  - E.g. vaddps, (vaddpd)



Basic Vectorization Switches

- Special switch for icx, Linux*, OS X*: **`-xHost`**
- Compiler checks SIMD features of current host processor (where built on) and makes use of latest SIMD feature available
- Code only executes on processors with same SIMD feature or later as on build host
- For AMD please check for the GNU flags e.g. **`-march=native`**

Please switch to icx/icpx/ifx Compiler!

- Deprecation of icc/ifort
- Check the user guide for supported flags:

  https://www.intel.com/content/www/us/en/docs/dpcpp-cpp-compiler/developer-guide-reference/2025-0/overview.htm

- Check results and compare with icc/icpc results:

  -fp-model=fast is the default

  -fp-model=precise might help to reproduce previous results

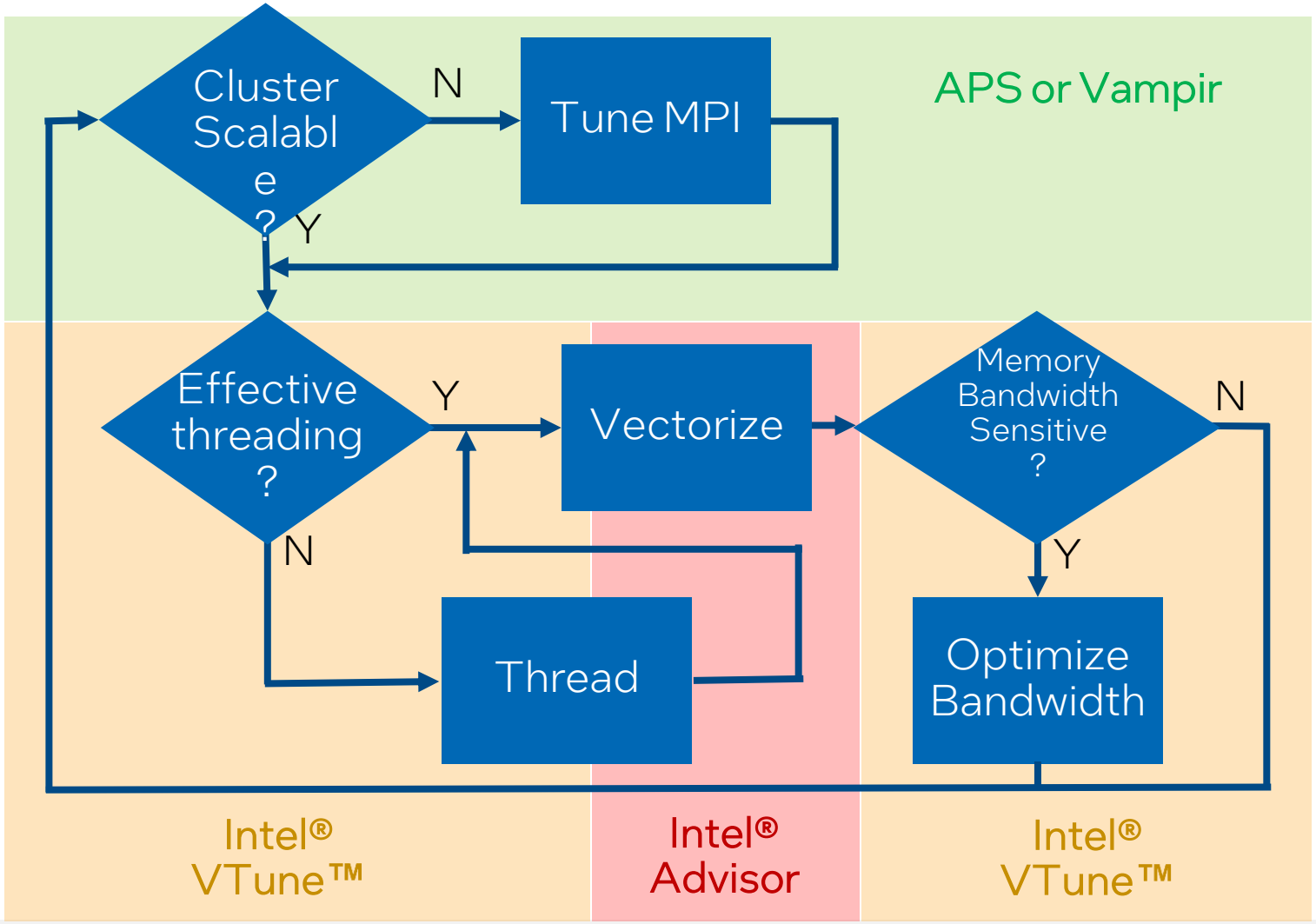
- Good flags to start with: -O2 -xhost

Online Resources

- Conformance to C/C++ standards – link
- GCC compatibility and interoperability – link
- Microsoft Visual C++ compatibility & Visual Studio integration – link
- Porting guide for *icc* users to *icx* – link
- C/C++/SYCL compiler forum – link

Which tool should I use?

Performance Analysis Tools for Diagnosis



Before dive to a particular tool..

- How to assess easily any potential in performance tuning?
- What to use on big scale not be overwhelmed with huge trace size, post processing time and collection overhead?
- Which tool should I use first?

- Answer: try Application Performance Snapshot (APS)

- Look for VTune module if available: **`$ module load VTune`**

APS Usage

Setup Environment

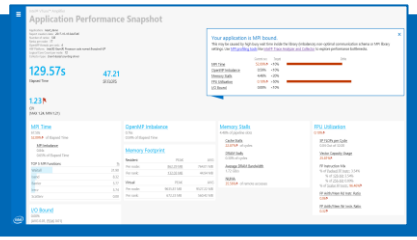
- $ source <path_to_vtune>/vtune_vars.sh # or load module

Run Application

- $ aps <application and args>
- MPI: $ mpirun <mpi options> aps <application and args>

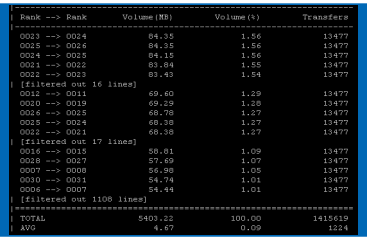
Generate Report on Result Folder

- $ aps –report <result folder>



Generate CL reports with detailed MPI statistics on Result Folder

- $ aps-report –<option> <result folder>



Application Performance Snapshot (APS)

Data in One Place: MPI+OpenMP+Memory Floating Point

Quick & Easy Performance Overview

- Does the app need performance tuning?

MPI & non-MPI Apps†

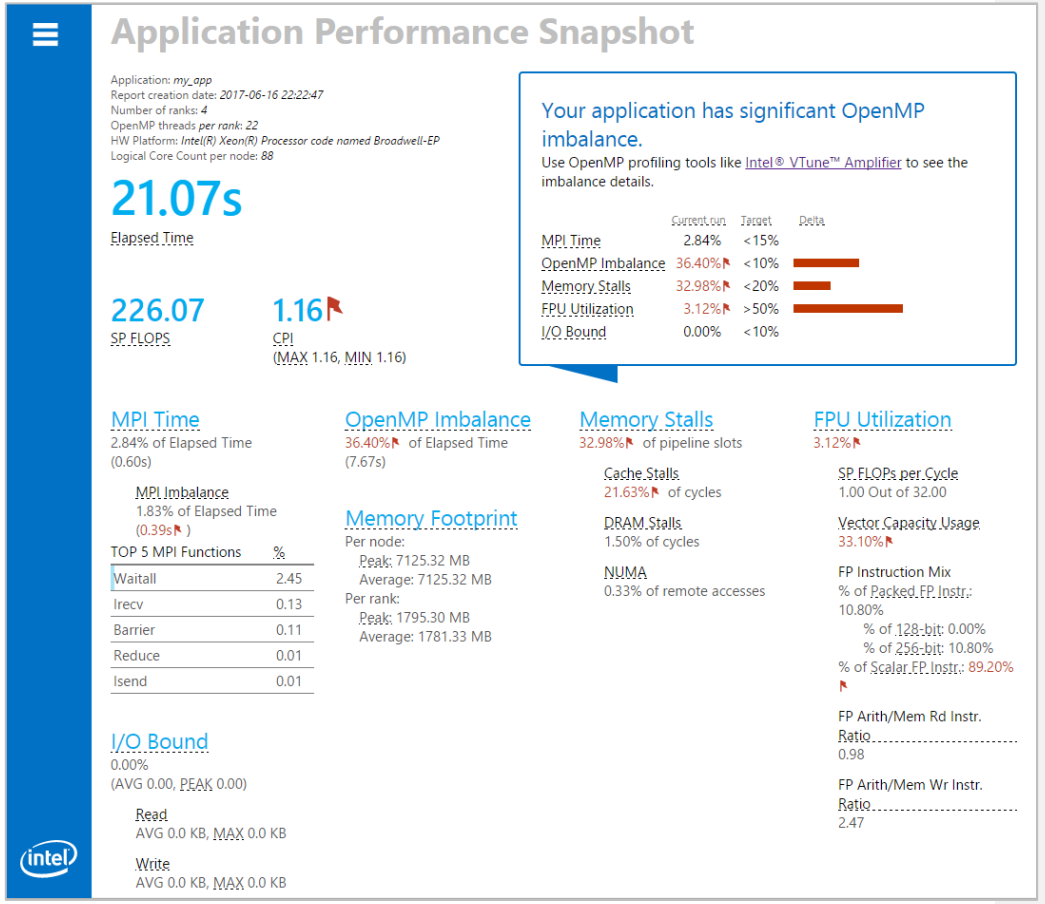
- Distributed MPI with or without threading
- Shared memory applications

Popular MPI Implementations Supported

- Intel® MPI Library
- MPICH & Cray MPI

Richer Metrics on Computation Efficiency

- CPU (processor stalls, memory access)
- FPU (vectorization metrics)



†MPI supported only on Linux*

APS Command Line Reports – Advanced MPI statistics

- Data Transfers for Rank-to-Rank Communication
  - aps-report –x <result>

And many others – check

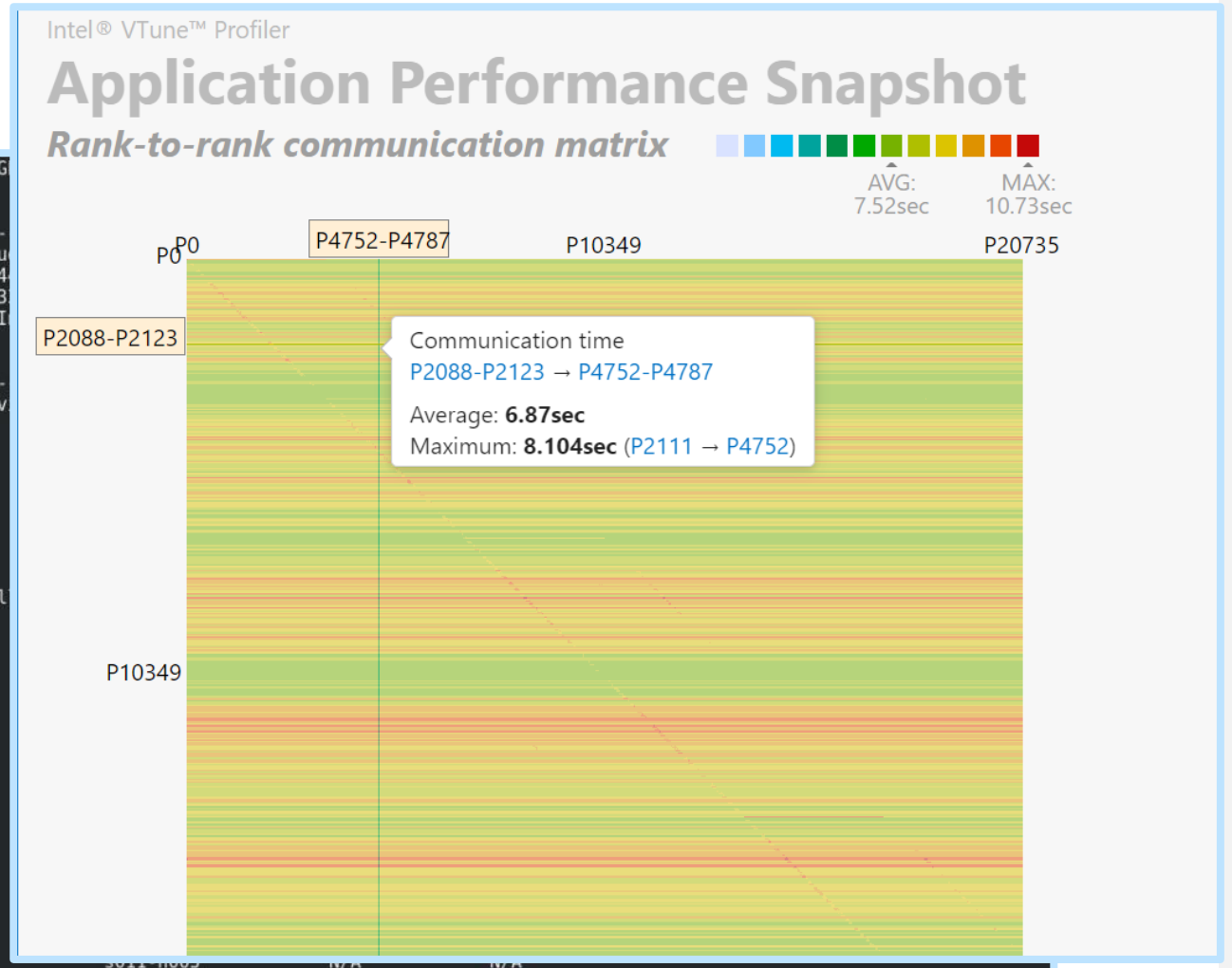
- aps-report -help

Rank --> Rank	Volume(MB)	Volume(%)	Transfers
0023 --> 0024	84.35	1.56	13477
0025 --> 0026	84.35	1.56	13477
0024 --> 0025	84.15	1.56	13477
0021 --> 0022	83.84	1.55	13477
0022 --> 0023	83.43	1.54	13477
[filtered out 16 lines]			
0012 --> 0011	69.60	1.29	13477
0020 --> 0019	69.29	1.28	13477
0026 --> 0025	68.78	1.27	13477
0025 --> 0024	68.38	1.27	13477
0022 --> 0021	68.38	1.27	13477
[filtered out 17 lines]			
0016 --> 0015	58.81	1.09	13477
0028 --> 0027	57.69	1.07	13477
0007 --> 0008	56.98	1.05	13477
0030 --> 0031	54.74	1.01	13477
0006 --> 0007	54.44	1.01	13477
[filtered out 1108 lines]			
TOTAL	5403.22	100.00	1415619
AVG	4.67	0.09	1224

Detailed reports

```
[root@nntpat98-144 aps_results]# aps --report -fDF
Loading 100.00%
| % - percentage of MPI functions total time
| Function summary for all Ranks
|-----------------------------------------------
|          Function             Time(sec)
|-----------------------------------------------
|             MPI_Waitall       972987.32
|                           Min: 0.0000
|                           Avg: 0.0001
|                           Max: 3.9528
|-----------------------------------------------
|             MPI_Allreduce     702927.29
|                           Min: 0.0000
|                           Avg: 0.0003
|                           Max: 1.8815
|-----------------------------------------------
|             MPI_Alltoallv     351070.07
|                           Min: 0.0000
|                           Avg: 0.0389
|                           Max: 17.3723
|-----------------------------------------------
|             MPI_Alltoall      178079.39
|                           Min: 0.0004
|                           Avg: 0.0030
|                           Max: 0.0197
|-----------------------------------------------
|             MPI_Barrier       105051.14
|                           Min: 0.0000
|                           Avg: 0.0650
|                           Max: 0.1494
|-----------------------------------------------
|             MPI_Isend         37178.85
|                           Min: 0.0000
|                           Avg: 0.0000
|                           Max: 0.2821
|-----------------------------------------------
|             MPI_Bcast         19726.74
|                           Min: 0.0000
|                           Avg: 0.0001
|                           Max: 1.4459
|-----------------------------------------------
|             MPI_Scatterv      8906.56
|                           Min: 0.0000
|                           Avg: 0.0015
|                           Max: 0.1564
|-----------------------------------------------
```

```
[root@nntpat98-144 aps_results]# aps --report --metrics="G
Loading 100.00%
| Metric Table
|-----------------------------------------------------------
Metric Name                         Node Name    Metric Valu
GPU Inbound PCIe Read, MB/s         s011-n004        207.14
GPU Inbound PCIe Read, MB/s         s011-n005        151.33
[root@nntpat98-144 aps_results]# aps --report --metrics="I
Loading 100.00%
| Metric Table
|-----------------------------------------------------------
Metric Name                                 Node Name    Dev
Inbound PCIe Read Per Device, MB/s          s011-n004
Inbound PCIe Read Per Device, MB/s          s011-n005
Inbound PCIe Read Per Device, MB/s          s011-n005
Inbound PCIe Read Per Device, MB/s          s011-n004
Inbound PCIe Read Per Device, MB/s          s011-n005
Inbound PCIe Read Per Device, MB/s          s011-n004
Inbound PCIe Read Per Device, MB/s          s011-n005
Inbound PCIe Read Per Device, MB/s          s011-n004
[root@nntpat98-144 aps_results]# aps --report --metrics=al
Loading 100.00%
GPU Time, s
GPU Time, s
GPU Time (% of Elapsed Time), % of Elapsed Time
GPU Time (% of Elapsed Time), % of Elapsed Time
GPU Utilization when Busy, %
GPU Utilization when Busy, %
GPU Occupancy, % of Peak Value
GPU Occupancy, % of Peak Value
GPU Inbound PCIe Read, MB/s
GPU Inbound PCIe Read, MB/s
GPU Inbound PCIe Write, MB/s
GPU Inbound PCIe Write, MB/s
GPU Outbound PCIe Read, MB/s
GPU Outbound PCIe Read, MB/s
GPU Outbound PCIe Write, MB/s
GPU Outbound PCIe Write, MB/s
Inbound PCIe Read Per Device, MB/s
Inbound PCIe Read Per Device, MB/s
Inbound PCIe Read Per Device, MB/s
```




```
s011-n004   N/A   GPU   Display controller: Intel Corporation De
s011-n005   N/A   GPU   Display controller: Intel Corporation De
s011-n005   N/A   GPU   Display controller: Intel Corporation De
```

APS potential issues

- If drivers are not available and for other hardware like AMD, you may use only mpi or/and openMP analysis (for Intel MPI):

```
$ aps --collection-mode=mpi[,openmp]
```

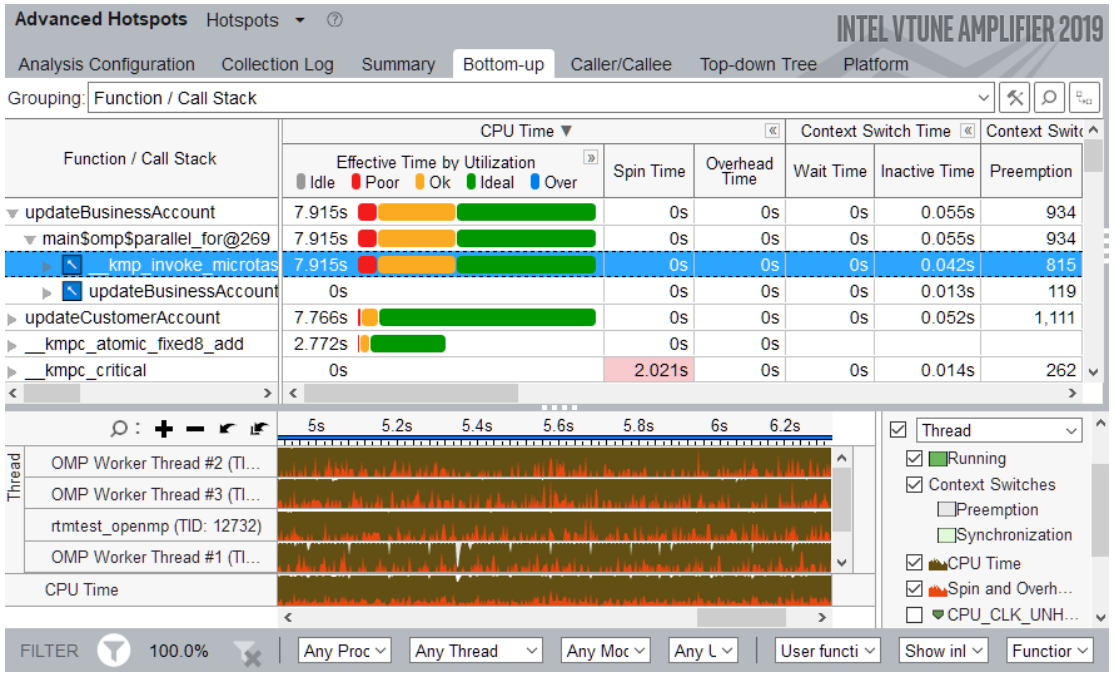
- If drivers are needed,you have to add this line to your batch job:

```
#SBATCH --disable-perfparanoid
```

Intel® VTune™ Profiler

Analyze & Tune Application Performance

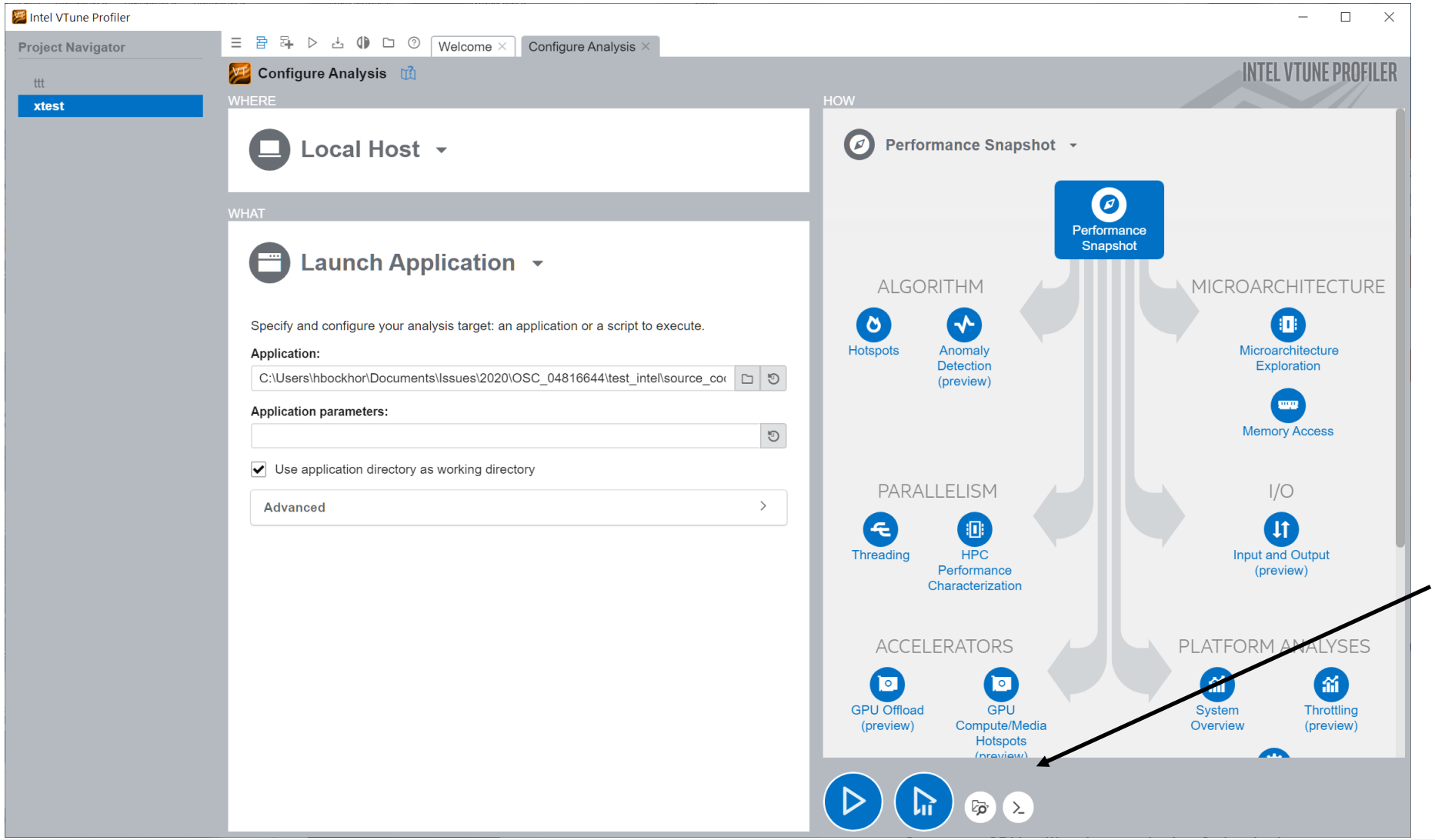
Intel® VTune™ Profiler



https://software.intel.com/content/www/us/en/develop/tools/vtune-profiler/get-started.html

- Accurately profile C, C++, Fortran*, Python*, Go*, Java*, or any mix
- Optimize CPU, threading, memory, cache, storage & more
- Take advantage of Priority Support
  - Connects customers to Intel engineers for confidential inquiries (paid versions)
- A more accessible user interface provides a simplified profiling workflow
- Smarter, faster Application Performance Snapshot: Analyze CPU utilization of physical cores, pause/resume, more... (Linux*)

Start a new Project



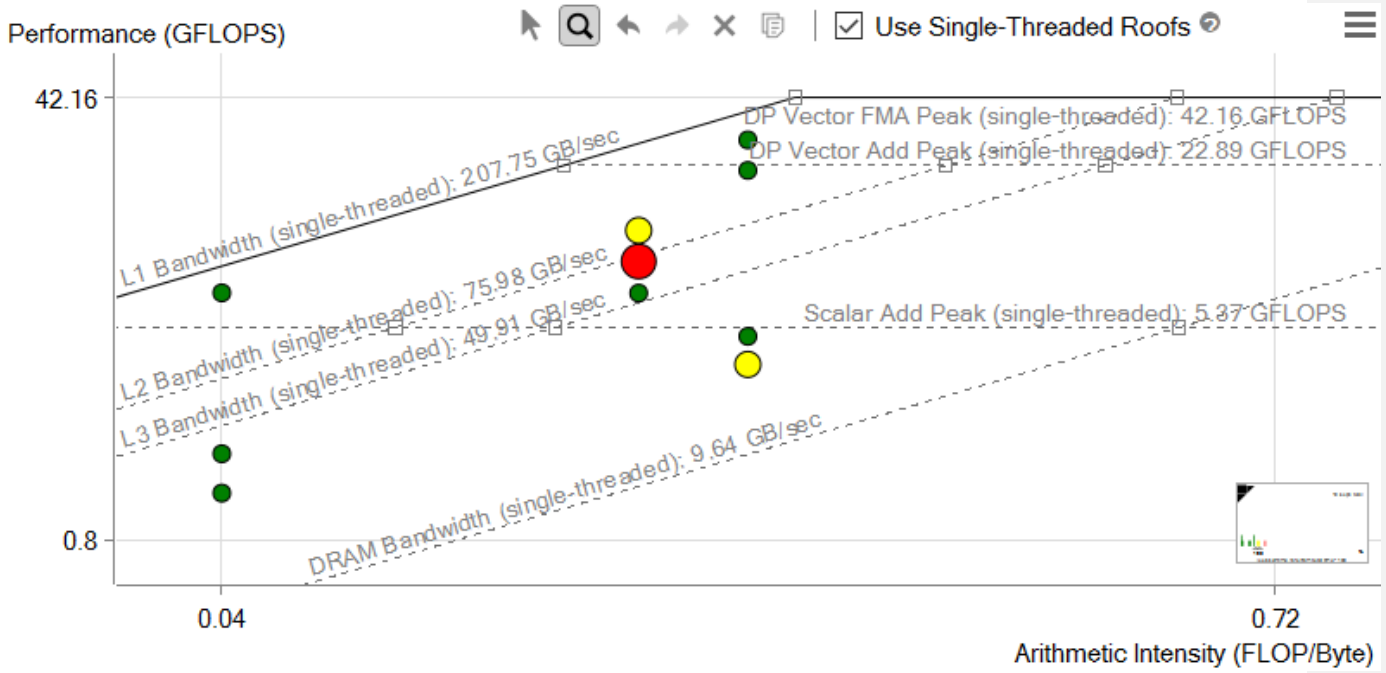
- Use GUI
- Or Command-Line

Get Command-Line

INTEL® ADVISOR

What is a Roofline Chart?

- A Roofline Chart plots application performance against hardware limitations.
  - Where are the bottlenecks?
  - How much performance is being left on the table?
  - Which bottlenecks can be addressed, and which *should* be addressed?
  - What's the most likely cause?
  - What are the next steps?



Roofline first proposed by University of California at Berkeley:
Roofline: An Insightful Visual Performance Model for Multicore Architectures, 2009
Cache-aware variant proposed by University of Lisbon:
Cache-Aware Roofline Model: Upgrading the Loft, 2013

Advisor + VTune Resources

Intel® Advisor

- Product page – overview, features, FAQs…
- What's New?
- Training materials – Cookbooks, User Guide, Tutorials
- Support Forum
- Online Service Center - Secure Priority Support

Additional Analysis Tools

- Intel® VTune™ Profiler – performance profiler

Additional Development Products

- Intel® oneAPI Toolkits

INTEL® MKL
INTEL® MPI

Intel oneMKL (Math kernel libraries)

- https://www.intel.com/content/www/us/en/developer/tools/oneapi/onemkl.html
- Math processing routines on CPU and GPU using C++, Fortran and python
- HPC and AI

Intel MPI

- https://www.intel.com/content/www/us/en/developer/tools/oneapi/mpi-library.html

- Is (Intel) GPU aware using device memory.

Intel Modules installed on Juwels/Jureca

▪ Compiler:	check available:	$ module spider Intel
	default:	$ module load Intel
▪ VTune + APS:	check available:	$ module spider vtune
	default:	$ module load VTune
▪ Advisor:	check available	$ module spider advisor
	default:	$ module load Advisor
▪ Intel MPI:	check available:	$ module spider intelMPI
	default:	$ module load IntelMPI
▪ Intel MKL:	check available:	$ module spider mkl
	default:	$ module load imkl


intel

How to start?

- Compile with minimal options and run with APS (will provide tuning tips)
- Compile with -O2 -xhost and and check timing and APS report
- Optional! Compile with –xhost and –no-vec
  disables vectorization. Compare with previous timing
- Use: VTune Profiler: $ module load VTune/<version>
- Use: Advisor: $ module load Advisor/<version> and create a roofline report.
- Google for Intel related topics → Intel Developer Zone etc.
- For APS/VTune add to your batch job: `#SBATCH --disable-perfparanoid`

- Please set thread affinity e.g.: $ export KMP_AFFINITY=scatter,verbose
  This can speed up OMP programs up to 10X!

- Any questions: Heinrich.Bockhorst@Intel.com

Basic Vectorization Switches I

- Linux*, OS X*: **-x<feature>**
  - Might enable Intel processor specific optimizations
  - Processor-check added to “main” routine:
    Application errors in case SIMD feature missing or non-Intel processor with appropriate/informative message
  - Example: -xCORE-AVX512 (Juwels Xeon SKL)

- Linux*, OS X*: **-ax<features>**
  - Multiple code paths: baseline and optimized/processor-specific
  - Multiple SIMD features/paths possible, e.g.: **-axSSE2,CORE-AVX512**
  - Baseline code path defaults to **-xSSE2**