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How to use Hunter

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Software environment



- Cray Programming Environment (CPE)
- As known from Hermit / Hornet / Hazel Hen
- Provides compilers:
 - Cray compiler (C/C++ compilers based on LLVM)

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- AMD compiler (LLVM-based)
- GNU
- provides highly optimized versions of BLAS/LAPACK, FFTW, Trilinos, HDF5, NetCDF
- Easy to switch between compilers (libs are automatically adapted)
- Furthermore provides debugger (gdb4hpc) and robust, comprehensive as well as easy-to-use performance analysis tools (perftools)

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- MI300A features "unified shared memory"
- i.e. CPU cores and GPU attached to same memory:
- → not necessary to copy data
- \rightarrow less effort and overhead
- \rightarrow allows *incremental* porting w/o sacrificing performance







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Programming models - HIP

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|--|---|--|
| CPU CODE | GPU CODE | APU CODE |
| double* in_h = (double*)malloc(Msize); double* out_h = (double*)malloc(Msize); | <pre>double* in_h = (double*)malloc(Msize); double* out_h = (double*)malloc(Msize); hipMalloc(∈_d, Msize); hipMalloc(&out_d, Msize);</pre> | <pre>double* in_h = (double*)malloc(Msize); double* out_h = (double*)malloc(Msize);</pre> |
| <pre>for (int i=0; i<m; cpu_func(in_h,="" i++)="" in_h[i]=";" initialize="" m);<="" out_h,="" pre=""></m;></pre> | <pre>for (int i=0; i<m; i++)="" initialize<br="">in_h[i] =; hipMemcpy(in_d,in_h,Msize); gpu_func<< >>(in_d, out_d, M); hipDeviceSynchronize(); hipMemcpy(out_h,out_d,Msize);</m;></pre> | <pre>for (int i=0; i<m; gpu_func<<="" i++)="" in_h[i]=";" initialize="">>(in_h, out_h, M); hipDeviceSynchronize();</m;></pre> |
| <pre>for (int i=0; i<m; cpu-process="out_h[i];</pre" i++)=""></m;></pre> | <pre>for (int i=0; i<m; cpu-process="out_h[i];</pre" i++)=""></m;></pre> | <pre>for (int i=0; i<m; cpu-process="out_h[i];</pre" i++)=""></m;></pre> |

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- GPU memory allocation on Device
- Explicit memory management between CPU & GPU
- Synchronization Barrier

The AMD Instinct MI300 APU Programming Model | Presented at ESPM2 at SC23 | AMD Public

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Programming models - OpenMP



OpenMP[®] CODE

#pragma omp requires unified_shared_memory double* in_h = (double*)malloc(Msize); double* out_h = (double*)malloc(Msize);

for (int i=0; i<M; i++) // initialize
 in_h[i] = ...;</pre>

#pragma omp target
{ ... }

for (int i=0; i<M; i++) // CPU-process
 ... = out_h[i];</pre>



Synchronous execution, but might be wise to use this opportunity to switch over to asychronous tasking approach (i.e. nowait clause)!

• GPU memory allocation on Device

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- Explicit memory management between CPU & GPU
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Programming models - stdpar

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C++

Fortran

std::transform(// needs <algorithm>
 std::execution::par_unseq, // <-- needs <execution>
 indices.begin(), indices.end(), grid.begin(),
 [](size_t index){
 return expensive_calculation(index);
 }

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);

Programming models - Compiler support

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|----------|---------|--------------|--------------|---------|---|--|--|--|--|
| Language | Model | | Compiler | | Comments | | | | |
| | | Cray | AMD | GNU | | | | | |
| Fortran | HIP | × | × | × | but possible via ISO_C_BINDING | | | | |
| | OpenMP | \checkmark | \checkmark | ? | GNU uses ROCm under the hood for OpenMP/OpenACC offloading. | | | | |
| | OpenACC | \checkmark | \checkmark | | MI300A not supported yet. But <i>might</i> be possible with recent enough ROCm. | | | | |
| | stdpar | \checkmark | | ? | not working yet (but should) | | | | |
| С | HIP | \checkmark | ✓ | × | Cray passes HIP sections to AMD compiler. Might be possible for GNU as well. | | | | |
| | OpenMP | \checkmark | \checkmark | ? | cf. Fortran | | | | |
| | OpenACC | × | × | × | | | | | |
| | HIP | \checkmark | \checkmark | × | cf. C | | | | |
| Cur | OpenMP | \checkmark | \checkmark | | cf. Fortran | | | | |
| C++ | OpenACC | × | × | × | | | | | |
| | stdpar | \checkmark | × | × | | | | | |
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Possible to mix them in your application

• \rightarrow allows for e.g. using OpenMP for majority of code but HIP in very hot kernels

But within a kernel / offloading unit, you can use a single model only.

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Need assistance?



- Join our "Hunter Code Preparation Workshop"
 - July 15th to 19th
 - hybrid
 - Port your workflow to CPE on Hawk & identify hot loops
 - AMD might shape porting efforts w.r.t. OpenFOAM, GROMACS, etc. based on your profile gathered in this workshop
 - https://www.hlrs.de/training/2024/hpe1
- Another workshop in November
 - test and improve your code on Hunter

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• More information will follow