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FRANCE 2030 PROGRAMME DE RECHERCHE *NUMÉRIQUE POUR L'EXASCALE*

Guix-Based Deployment and Unified Multi-GPU Support for NumPEx Proxy-Apps

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General Assembly Exa-DI

Plan

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Guix developments

Our Guix-channel: `guix-numpex`

The CDT uses Guix as its primary tool for deploying and managing the PC5 proxy-application stack.

`https://gitlab.inria.fr/numpex-pc5/guix-numpex`

`guix-numpex` channel

- Includes most of the applications involved in GT 1-3
- Reproducible, traceable builds across HPC platforms

Apologize to Enabling Team : we will contribute to Guix-science ...

Packaged Applications Across Working Groups

Working Group	Packaged Applications
GT1 - High Order Schemes	proxy-GEOS, proxy-FUn (CUDA & HIP)
GT2 - Unstructured Mesh	Arcane, Sharc
GT3 - Block-structured AMR	Dyablo (AthenaK and/or Castro coming soon)

Focus: proxy-GEOS and multiplication of configurations

What is proxy-GEOS?

Proxy application for wave propagation simulations (2D/3D acoustic wave equation)

- Multiple programming models: OpenMP, RAJA, **Kokkos**
- Supported on AMD & Nvidia GPUs

The packaging challenge

Goal: Provide ready-to-use packages covering all configurations

- GPU backends (CUDA, HIP) $\times$ architectures (V100, A100, MI250...)
- Users should not need package transformations or manual tweaks
- Combinatorial explosion of package variants

$\Longrightarrow$ Exploration of multiple GPU applications

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Multiple GPUs application

Nvidia GPUs Binary Compatibility

No binary compatibility across GPU generations

A binary compiled for one GPU architecture will not run on another generation

- Different instruction sets and capabilities
- Example: V100 (Volta) $\not\to$ A100 (Ampere) $\not\to$ H100 (Hopper)

Within-generation compatibility

Limited forward-compatibility within the same generation

- Example: A100 binary $\to$ A6000 (both Ampere)

Question: How to build once and support multiple generations?

Step 1: Virtual Architecture

What is a virtual architecture?

- **Not an actual GPU architecture**
- Defines a set of generic instructions and capabilities
- Used to generate **PTX assembly** (Parallel Thread Execution)

Role in compilation

PTX serves as intermediate representation to build application binaries for specific GPU architectures

Syntax

```
--gpu-architecture=compute_XX
```

- Example: `compute_80` for Ampere generation

Step 2: JIT or multiple CUDA Binaries Mechanism

The GPU compatibility mechanism depends on **when** the real architecture is specified.

multiple CUDA Binaries (cubins) (compile-time)

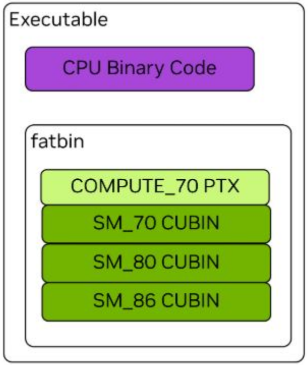
- Generate multiple binary versions at compile time
- One specific binary per targeted GPU model
- Real GPU architectures must be known at compile time

Just-In-Time (JIT) Compilation (runtime)

- GPU code generated at runtime when driver detects the architecture
- Induces startup overhead (mitigated by caching)
- Forward-compatible with future GPU models

Note: Both mechanisms can be combined (hybrid approach)

Fat Binary Structure



Source: NVIDIA Developer Blog
`https://developer.nvidia.com/blog/understanding-ptx-the-assembly-language-of-cuda-gpu-computing/`

What's inside?

- CPU binary code (host)
- Multiple CUBINs for targeted architectures
- PTX for JIT compilation
- Driver selects appropriate code at runtime

Compilation Setup for Binary compatibility support

Two key compilation options

`--gpu-architecture`: virtual architecture (Step 1)
`--gpu-code`: real architecture(s) or virtual for JIT (Step 2)

Example 1: Forward-compatible within generation

```
nvcc --gpu-architecture=compute_80 --gpu-code=sm_80 x.cu -o x.exe
```

Works on: A100 (sm_80), A6000 (Ampere 8.0+) — Fails on: V100 (older gen), H100 (no JIT)

Example 2: Hybrid (CUDA binary + JIT)

```
nvcc --gpu-architecture=compute_80 --gpu-code=sm_80,compute_80 x.cu
```

Works on: A100 (sm_80), H100 (sm_90) with JIT — Fails on: V100 (older gen)

Toy Use-Case: Matrix-Vector Multiplication

Testing methodology

Simple CUDA kernel to benchmark compilation mechanisms

- Matrix-vector product: 1000×1000 matrix
- Execution time averaged over 100 runs
- Tested on Ada (sm_89) GPU with CUDA 12.4

CUDA kernel

```
__global__ void mat_vect_prod(
    float* mat, float* vec,
    float* res, int n, int m) {
  int idx = blockIdx.x * blockDim.x
            + threadIdx.x;
  if (idx < n) {
    for (int i = 0; i < m; i++)
      res[idx] += mat[m*idx+i]
                  * vec[i];
  }
}
```

Comparison metrics

- Executable size
- Runtime performance
- Impact of multiple cubins vs JIT

multiple CUDA Binary: Results

Configuration	--gpu-arch	--gpu-code	Size	Time (s)
Fat80	compute_80	sm_80	812K	0.125
Fat89	compute_89	sm_89	812K	0.122
Fat80/80-86-89	compute_80	sm_80,sm_86,sm_89	824K	0.132
Fat80-86-89	compute_80	sm_80	824K	0.128
	compute_86	sm_86		
	compute_89	sm_89		

- Multiple architectures increase binary size slightly (+12K)
- Best performance obtained for the specific build of Ada89 (Fat89)
- Performance remains consistent across configurations

JIT Compilation: Results

Configuration	--gpu-arch	--gpu-code	Size	Time (s)	Time (s)[1]
JIT80	compute_80	compute_80	808K	0.134	0.14
JIT89	compute_89	compute_89	808K	0.137	0.15
JIT80 + Fat80/89	compute_80	compute_80, sm_89	812K	0.123	0.14
JIT89 + Fat89	compute_89	compute_89, sm_89	812K	0.12	0.136
JIT70 + Fat70/89	compute_70	compute_70, sm_89	812K	0.14	0.144
JIT70+Fat70/89 +	compute_70	compute_70, sm_89	824K	0.123	0.1375
JIT80+Fat80/89	compute_80	compute_80, sm_89			

[1] Cache disabled + JIT forced

Key observations

- Executable sizes remain constant among several configurations
- Execution times remain constant among several configurations
- JIT caching is effective (uncached: +5-10% overhead)

Application to proxy-GEOS

From toy example to real application

The multi-GPU mechanisms apply to the full proxy-GEOS stack

- Configure `CMAKE_CUDA_ARCHITECTURES` with explicit list: `70;80;86;89` $\Longrightarrow$ Hybrid approach using multiple cubins & JIT.
- Use GPU compiler (nvcc/hipcc) as main compiler
- Enable corresponding CMake language (CUDA or HIP)
- **Third-Party Libraries** (Kokkos, Raja,etc.) must also support multi-GPU compilation
  - Available features in Raja
  - Patched manually in Kokkos (No details given here)

proxy-GEOS: Test Configurations

Goal: Benchmark multi-GPU support on V100 (7.0) and A100 (8.0)

Test configurations

- `Hybrid70`: V100-based (`CMAKE_CUDA_ARCHITECTURES=70`) with JIT fallback
- `Hybrid80`: A100-based (`CMAKE_CUDA_ARCHITECTURES=80`) with JIT fallback
- `all-major_80`: All major architectures up to 8.0 (`CMAKE_CUDA_ARCHITECTURES="50;60;70;80"`)
- `all_86`: All architectures up to 8.6 (`CMAKE_CUDA_ARCHITECTURES="50;52;53;60;61;62;70;72;75;80;86"`)

proxy-GEOS: Benchmark Results

Config	Size	V100 (no cache)	A100 (no cache)	V100 (cached)	A100 (cached)
Hybrid80	3.2M	N/A	4.02s	N/A	2.51s
Hybrid70	3.2M	5.24s	4.08s	3.75s	2.54s
all-major_80	5.2M	5.21s	4.04s	3.75s	2.57s
all_86	9.9M	5.23s	4.04s	3.73s	2.60s

- Binary size increases with more architectures (3.2M $\rightarrow$ 9.9M)
- JIT caching reduces runtime by 30%
- Performance remains consistent across multi-GPU configurations

Impact on Guix Packaging

Before: Multiple packages

- `proxy-geos-kokkos-cuda-v100`
- `proxy-geos-kokkos-cuda-a100`
- `proxy-geos-kokkos-cuda-a40`
- `proxy-geos-kokkos-cuda-ada`
- `proxy-geos-kokkos-cuda-h100`

After: Single unified package

- `proxy-geos-kokkos-cuda-all`

```
Fatbin elf code:
arch = sm_75
arch = sm_80
arch = sm_86
arch = sm_89
arch = sm_90
```

Solution: One package, multiple GPUs supported

Result: Easy deployment for users, reduced maintenance for developpers

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Conclusion

Conclusion

Multi-GPU build: Lessons learned

- Hybrid multiple cubins + JIT approach balances performance and flexibility
- One package replaces dozens of architecture-specific variants
- Extend the work for AMD GPUs

guix-numpex channel: Next steps

- Contribute back to **Guix-Science** channel

Thank you for your attention. Any Questions?

https://numpex-pc5.gitlabpages.inria.fr/wp2-co-design/doc-hub/multigpus-build/index.html

Appendix: Kokkos Patches for Multi-GPU Support

Why patch Kokkos?

Native Kokkos (v4.6.1) did not support multiple GPU architectures when using `KOKKOS_ENABLE_COMPILE_AS_CMAKE_LANGUAGE`

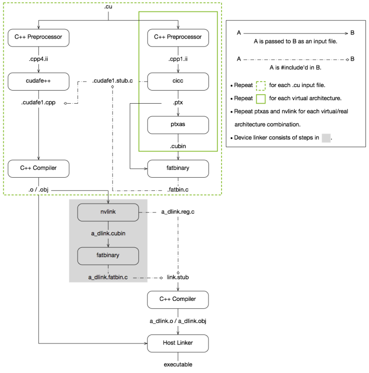
Key modifications in `kokkos_arch.cmake`:

- **Allow multiple architectures:** Remove fatal error when multiple `KOKKOS_ARCH_XX` are specified
- **Build architecture list:** Append architectures to `KOKKOS_CUDA_ARCHITECTURES` instead of overwriting
- **Propagate to CMake:** Set `CMAKE_CUDA_ARCHITECTURES` with semicolon-separated list

Additional fix in `Kokkos_DesulAtomicsConfig.hpp`:

- Define `KOKKOS_ARCH_XXX` macros based on runtime `__CUDA_ARCH__`
- Enables architecture-specific code paths within kernels

Appendix: Cuda compilation



CUDA Compilation Trajectory

Source: NVIDIA Documentation
`https://docs.nvidia.com/cuda/cuda-compiler-driver-nvcc/`