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Systematically Exploring High-Performance Representations of Vector Fields Through Compile-Time Composition

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Introduction: Vector Fields

- Vector fields map vectors onto elements of a set
- Common case: mapping vectors onto structured grids

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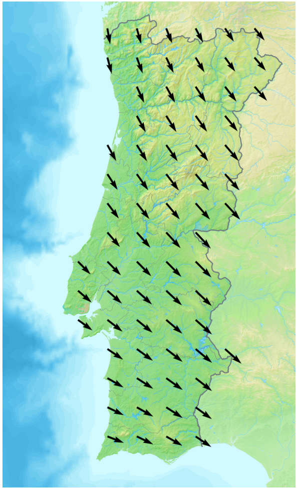
- Useful for modelling flows like wind...



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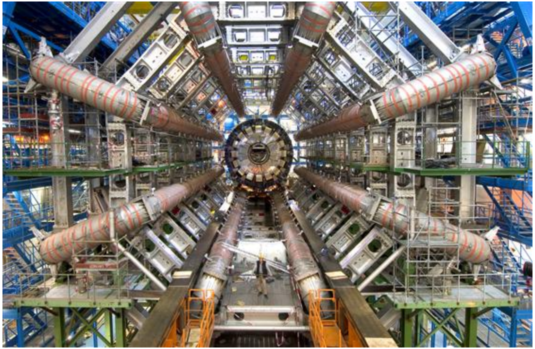
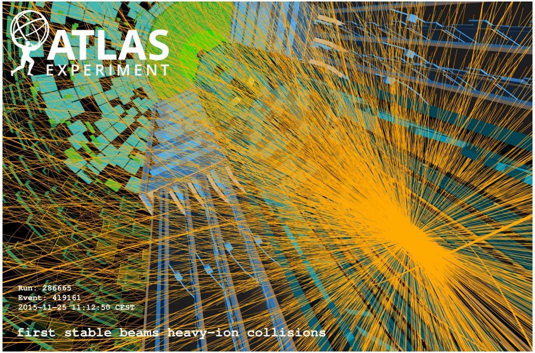


Credit: ATLAS Collaboration

Introduction: Vector Fields

- Vector fields map vectors onto elements of a set
- Common case: mapping vectors onto structured grids
- Useful for modelling flows like wind...
- ...or magnetic fields in high-energy physics



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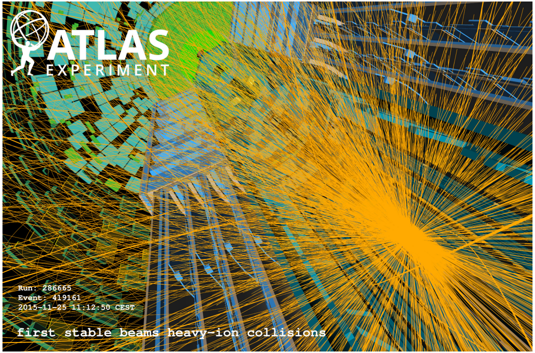
Introduction: Vector Fields

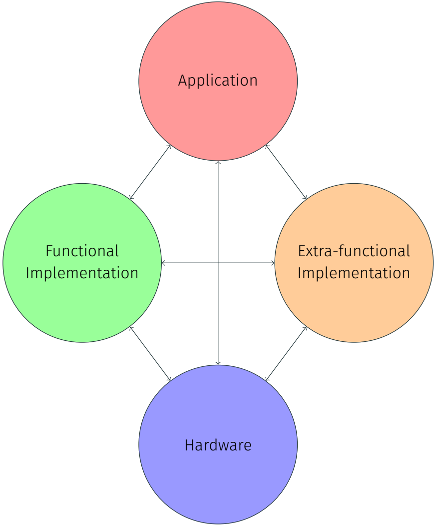
- Vector fields map vectors onto elements of a set
- Common case: mapping vectors onto structured grids
- Useful for modelling flows like wind...
- ...or magnetic fields in high-energy physics
- Performance-relevant data structures, but which representation is best?



Credit: ATLAS Collaboration

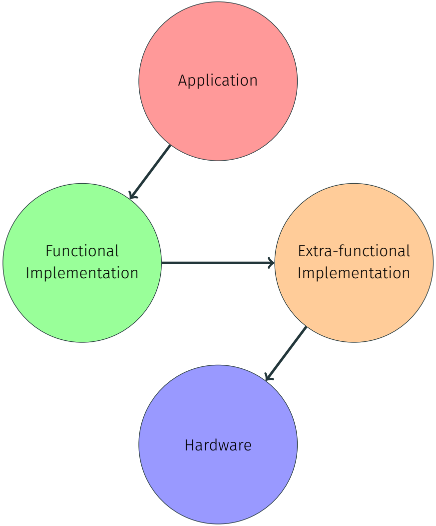
Design Space Definition

- Large design space: performance depends heavily on the *interaction between*:
    - Application
    - Functional implementation
    - Extra-functional implementation
    - Hardware



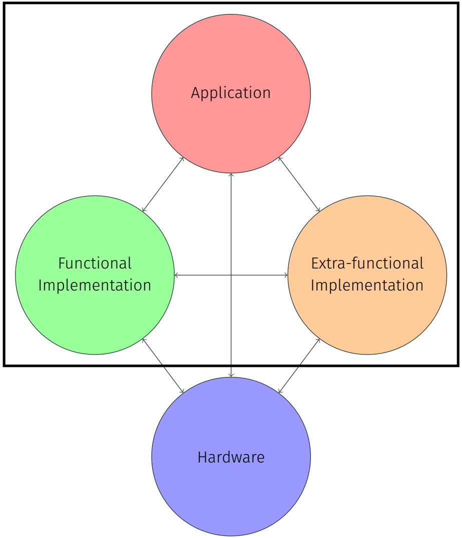
Design Space Definition

- Example: application migrates from two-dimensional approximation to three-dimensional field:
  - Functional implementation of the field changes…
  - …the storage size changes (extra-functional behaviour)…
  - …and the hardware cache behaviour changes



Design Space Exploration

- Our goal: allow systematic exploration of representations of vector fields
    - *Define* the design space
    - *Compose* representations from simple components
    - Facilitate exploration through *benchmarking*



Application: Access Patterns

- In our suite, *applications* are modelled by their *access patterns*, capturing:
  - Locality of access
  - Computational side-effects
  - Functional requirements
- Variants:
  - CPU and GPGPU implementations
  - For patterns based on propagation through fields: order of execution
  - Depth-first or breadth-first propagation of agents

Name	Vr.	Field type
SCAN	2	$\prod_{d,d':\mathbb{N}} S^{d+d'} \to T$
RANDOM	2	$\prod_{d:\mathbb{N}} S^{d} \to T$
EULER	3	$\prod_{d:\mathbb{N}} \mathbb{R}^{d} \to \mathbb{R}^{d}$
RK4	3	$\prod_{d:\mathbb{N}} \mathbb{R}^{d} \to \mathbb{R}^{d}$
LORENTZ	6	$\mathbb{R}^{3} \to \mathbb{R}^{3}$

Implementation: Storage Backends

- Implementation of field data structure remains dauntingly complex
- Many choices of implementation
  - Functional: interpolation, boundary checking, geometric transformations, etc.
  - Extra-functional: data layouts, hardware acceleration, etc.
- This behaviour can (must!) be further decomposed into *primitive* behaviour and *transformers*

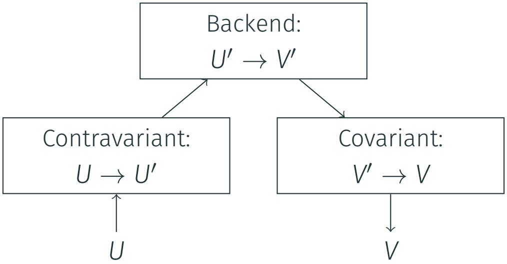
Implementation: Primitive Storage

- Behaviour that cannot be meaningfully deconstructed
  - Basic array access (Array, CudaArray)
  - More complex storage like CUDA textures (CudaTex) or opaque arrays (CudaPitch)
  - Constant-valued and analytical fields (Constant, Analytical)

Name	Pltf.	Field type
Array	CPU	$\mathbb{N} \to T$
CudaArray	CUDA	$\mathbb{N} \to T$
CudaPitch	CUDA	$\prod_{d:[\![1,3]\!]} \mathbb{N}^d \to T$
CudaTex	CUDA	$\prod_{d:[\![1,3]\!]} \prod_{d':[\![1,4]\!]} \mathbb{R}^d \to \mathbb{R}^{d'}$
Analytic	CPU	$S \to T$
Constant	Any	$S \to T$

Implementation: Transformers

- Additional behaviour encoded as *transformers*, built of two parts:
    - *Contravariant* component allows to *modify input*
    - *Covariant* component allows to *modify output*



Implementation: Transformers

```
float[3] backend(uint i) {
    return arr[i];
}
```

```
uint contravar(uint c[3]) {
    return c[0] + N[0] *
        (c[1] + N[1] * c[2]);
}
```

$\mathbb{N}^3$

```
float[3] covar(float[3] v) {
    return v;
}
```

$\mathbb{R}^3$

Implementation: Transformers

```
float[3] backend(uint i) {
    return arr[i];
}
```

```
uint contravar(uint i) {
    return i;
}
```

```
float[2] covar(float[3] v) {
    return {v[0], v[1]};
}
```

$\mathbb{N}$

$\mathbb{R}^2$

Implementation: Transformers

```
float[3] backend(uint i) {
    return arr[i];
}
```

```
uint contravar(uint c[3]) {
    return c[0] + N[0] *
        (c[1] + N[1] * c[2]);
}
```

```
uint[3] contravar(float c[3]) {
    return {round(c[0],
    round(c[1]), round(c[2])};
}
```

$\mathbb{R}^3$

```
float[3] covar(float[3] v) {
    return v;
}
```

```
float[3] covar(float3 v) {
    return v;
}
```

$\mathbb{R}^3$

Implementation: Transformers

- We provide a variety of transformers for common implementation details
- These can be composed as long as the types line up
- Many transformers have additional variants (e.g. Wrap)

Name	Type
Lexic.	$\prod_{n:\mathbb{N}}(\mathbb{N}^n \to \mathbb{N}) \times (T \to T)$
Morton	$\prod_{n:\mathbb{N}}(\mathbb{N}^n \to \mathbb{N}) \times (T \to T)$
Hilbert	$(\mathbb{N}^2 \to \mathbb{N}) \times (T \to T)$
Shuffle	$\prod_{n:\mathbb{N}}\prod_{p:\mathfrak{S}_n}(S^n \to S^n) \times (T \to T)$
OOB	$(S \to S + \mathbb{1}) \times (T + \mathbb{1} \to T)$
Wrap	$(S \to S) \times (T \to T)$
Nearest	$\prod_{n:\mathbb{N}}(\mathbb{R}^n \to \mathbb{N}^n) \times (T \to T)$
Linear	$\prod_{n:\mathbb{N}}(\mathbb{R}^n \to \mathbb{N}^{2^n n} \times \mathbb{R}^n) \times (\mathbb{R}^{2^n n} \times \mathbb{R}^n \to \mathbb{R}^n)$
Affine	$\prod_{n:\mathbb{N}}(\mathbb{R}^n \to \mathbb{R}^n) \times (T \to T)$

Benefit: Extensibility

- New access pattern has “free” benchmarks with hundreds of backends
- New primitive storage composes with many transformers
- New transformer is compatible with many access patterns

Composition in High-Performance Kernels

- Composition is usually achieved through run-time polymorphism
- Incurs overhead from dynamic function dispatch
- Manageable for most applications…
- …but deal-breaking in HPC kernels

```
backend f1;
layer3 f2(f1);
layer2 f3(f2);
layer1 f4(f3);

vector3 v = f4.at(5.f, 2.f, -2.f);
```

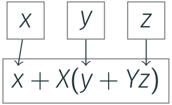
Compile-Time Composition

- Instead of composing at *run-time*, we compose behaviour at *compile-time*
- Use of C++ templating fixes behaviour at compile-time
    - Eliminates overhead due to dispatching
    - Increases optimisation space of the compiler
- We achieve native performance *and* preserve flexibility

```
using storage = layer1<
    layer2<
        layer3<
            backend<...>
        >,
        ...
    >,
    ...
>;
```

Compile-Time Composition

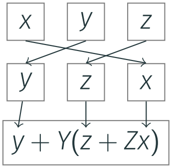
```cpp
using storage = lexicographic<ulong3,
      ulong3>;
```




```asm
; g++ 12.2.0 x86_64_v1
imul    0x8(%rsi),%rdx
add     %rcx,%rdx
imul    0x10(%rsi),%rdx
add     %rdx,%r8
mov     0x18(%rsi),%rdx
lea     (%r8,%r8,2),%rax
lea     (%rdx,%rax,8),%rax
movdqu  (%rax),%xmm0
mov     0x10(%rax),%rax
movups  %xmm0,(%rdi)
mov     %rax,0x10(%rdi)
mov     %rdi,%rax
ret
```

Compile-Time Composition

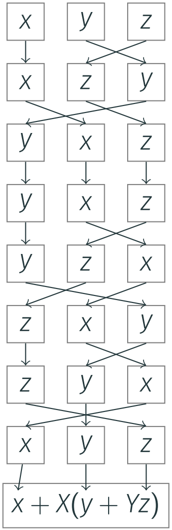
```cpp
using storage = shuffle<lexicographic
    <ulong3, ulong3>, perm<1, 2, 0>>;
```




```asm
; g++ 12.2.0 x86_64_v1
imul    0x8(%rsi),%rcx
add     %r8,%rcx
imul    0x10(%rsi),%rcx
lea     (%rcx,%rdx,1),%rax
mov     0x18(%rsi),%rdx
lea     (%rax,%rax,2),%rax
lea     (%rdx,%rax,8),%rax
movdqu  (%rax),%xmm0
mov     0x10(%rax),%rax
movups  %xmm0,(%rdi)
mov     %rax,0x10(%rdi)
mov     %rdi,%rax
ret
```

Compile-Time Composition

```cpp
using storage = shuffle<shuffle<
      shuffle<shuffle<shuffle<shuffle<
      shuffle<lexicographic<ulong3,
      ulong3>, perm<2, 1, 0>>, perm<0,
      2, 1>>, perm<1, 2, 0>>, perm<0,
      2, 1>>, perm<0, 1, 2>>, perm<2,
      0, 1>>, perm<0, 2, 1>>;
```




```asm
; g++ 12.2.0 x86_64_v1
imul    0x8(%rsi),%rdx
add     %rcx,%rdx
imul    0x10(%rsi),%rdx
add     %rdx,%r8
mov     0x18(%rsi),%rdx
lea     (%r8,%r8,2),%rax
lea     (%rdx,%rax,8),%rax
movdqu  (%rax),%xmm0
mov     0x10(%rax),%rax
movups  %xmm0,(%rdi)
mov     %rax,0x10(%rdi)
mov     %rdi,%rax
ret
```

Empirical Evaluation (HEP Example): Setup

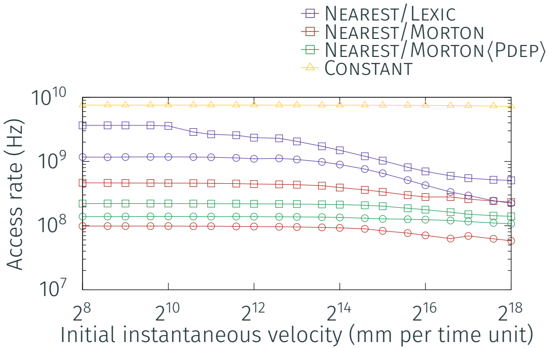
- We imagine a high-energy physicist
- Goal: find the best implementation of a vector field in her software
- Select one of the access patterns that models the application
    - Not exactly the same as the real application, but sufficiently close
- Make a selection of candidate implementations
    - Construct these from the “building blocks” discussed before
- This generates a set of benchmarks, which can be run on one or more systems
- In this case: six setups in the DAS-6[1] compute cluster!

[1] *https://www.cs.vu.nl/das6/*

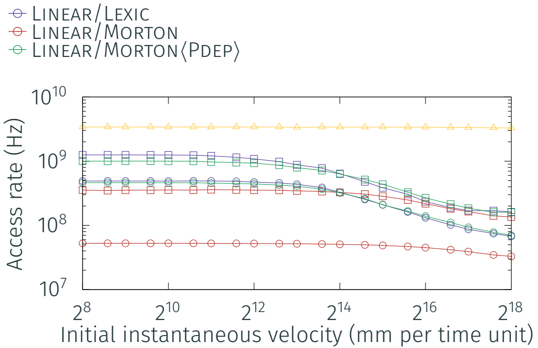
Empirical Evaluation (HEP Example): Setup

```
benchmark::register_product_bm<
    // Seven access patterns
    boost::mp11::mp_list<
        Lorentz<Euler>,
        Lorentz<RungeKutta4>,
        RungeKutta4Pattern,
        EulerPattern,
        Random,
        Scan>,
    // Seven composite implementations
    boost::mp11::mp_list<
        FieldConstant,
        FieldTex<TexInterpolateLin>,
        FieldTex<TexInterpolateNN>,
        Field<InterpolateNN, LayoutStride>,
        Field<InterpolateNN, LayoutMorton>,
        Field<InterpolateLin, LayoutStride>,
        Field<InterpolateLin, LayoutMorton>
    >
    // Generates a large number of benchmarks!
>();
```

Empirical Evaluation (HEP Example): Results

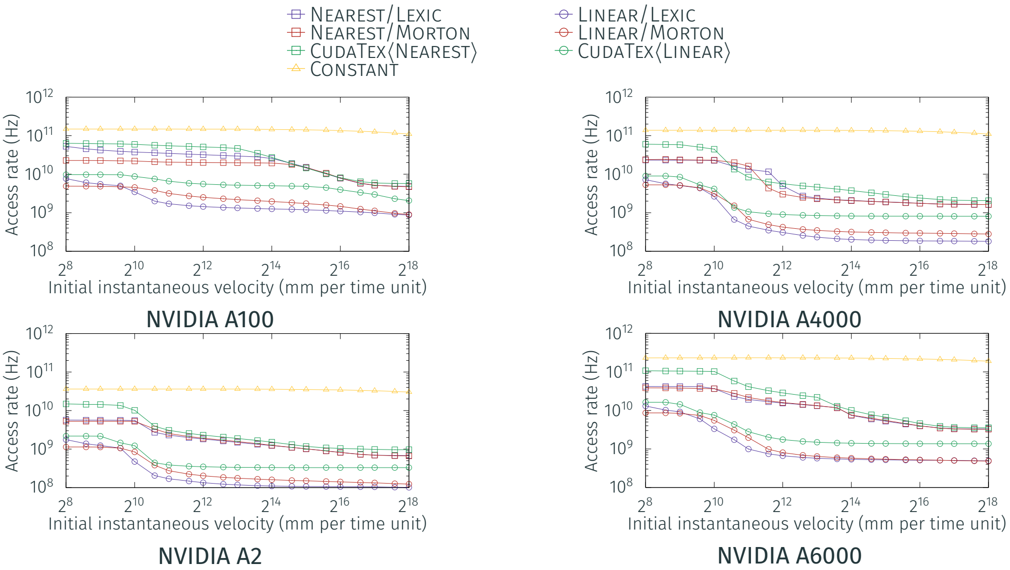


AMD EPYC 7402P (48 threads)



Intel Xeon E5-2630 v3 (2 sockets, 32 threads)

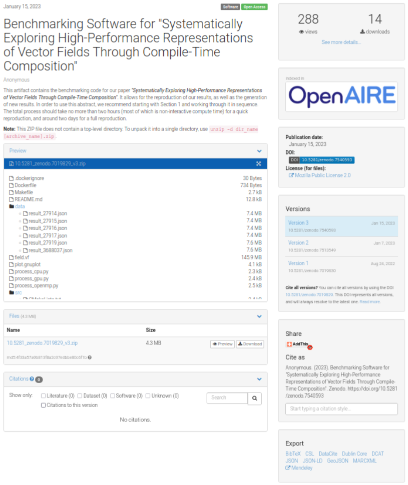
Empirical Evaluation (HEP Example): Results



Usage in Real-World Applications

- Our benchmark suite provides a range of components and infrastructure
- This translates (with some effort on our part) to a *user-facing library*
- Makes the results of benchmarks immediately *applicable*
- Eliminates ambiguity between benchmark results and manual re-implementation
- Library available under MPL-2.0 license
- Currently in use in experimental HEP software!

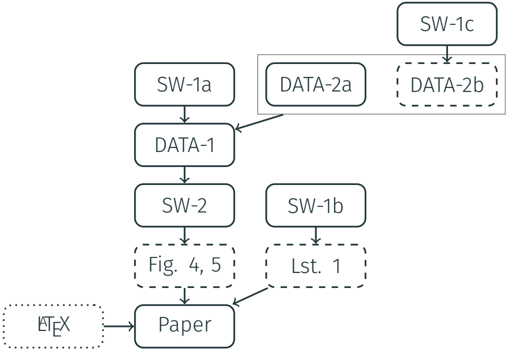
Artifact



- Artifact is permanently available at *`https://zenodo.org/record/7540593`*
- Provided with an *optional* Docker file
- Specific care taken to ensure code works without Docker
    - But using the Docker file will guarantee sane and reproducible environment

Artifact

- SW-1 Benchmarking suite:
  - a Primary benchmarking code
  - b Code for assembly inspection
  - c Dummy field generation code
- SW-2 Plotting code.
- DATA-1 Results from our experiments
- DATA-2 Vector field data
  - a Real-world data from HEP
  - b Dummy field data



Conclusion

- We present a *benchmark suite* for vector fields on structured grids
- *Composition* at compile-time achieves native performance while being *extensible* and allowing *design space exploration*
- Gives rise to a *novel library*, available publicly now
- *Artifact* available to fully reproduce our results, and to generate new data