Empowering Domain Experts through Automatic Code Transformation of HPC Kernels

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HPC Environment

- Today's HPC architecture:
  - Distributed many-core systems
  - Accelerators
  - High-speed interconnection
  - Separated IO servers for parallel file system
- Popular tools
  - Parallelisation on shared memory: OpenMP
  - Parallelisation on shared memory: MPI
  - Self-describing scientific data format: netCDF

"The questions don't change, the answers do" – *Daniel Reed*

Solving the Problem

Domain experts' situation:

- More complex computer science skills required [AC16]
- HPC skills underrepresented [MHS+20]
- Support by application software engineers sometimes possible
  - about 80 000 €/yr

Solution approach provided by CATO [SJB+20]

- Partitioning relevant memory
- Optimise netCDF usage: chunking, parallel IO, compression
- `https://github.com/JSquar/cato`

LLVM Infrastructure

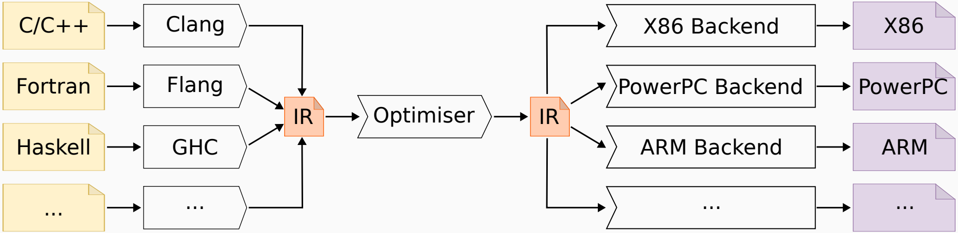


Figure 1: Modular LLVM infrastructure (based on [Lat]).

CATO Pass

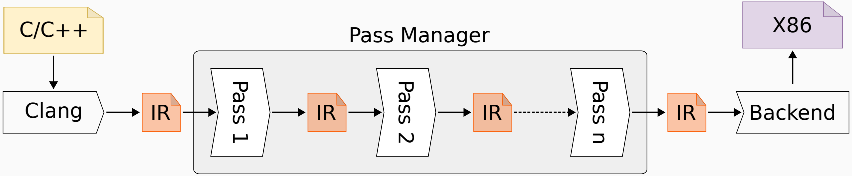


Figure 2: Insertion of CATO Pass (based on [Sam15]).

- `EP_ModuleOptimizerEarly`
- Load pre-compiled C++ replacement code as LLVM module
- Find relevant code instructions (OpenMP kernels)
- Perform modification

Memory Distribution

Memory Access Pattern

- 7+6 Dwarves [Col04, ABC+06]
- Nature is (usually) local $\rightarrow$ Stencil

$$
\begin{aligned}
f(x,y) =& C + a_0 \cdot f(x,y) \\
& + a_1 \cdot f(x-1,y) + a_2 \cdot f(x+1,y) \\
& + a_3 \cdot f(x,y-1) + a_4 \cdot f(x,y+1)
\end{aligned}
$$

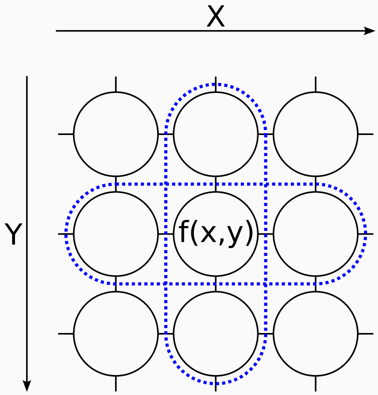


Figure 3: 5-point stencil

Stencil Distribution

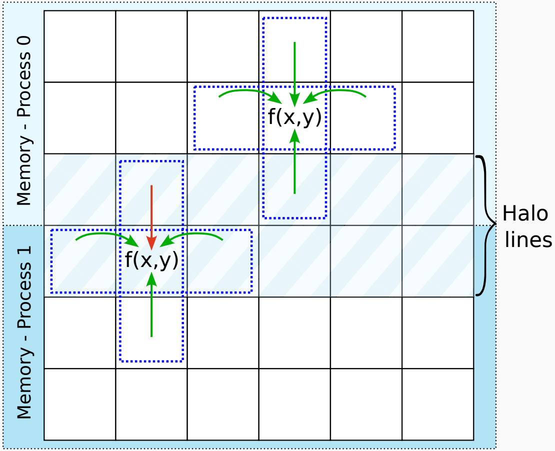


Figure 4: Green arrows: local memory. Red arrows: neighbouring process

Improved Memory Consumption - Runtime Data

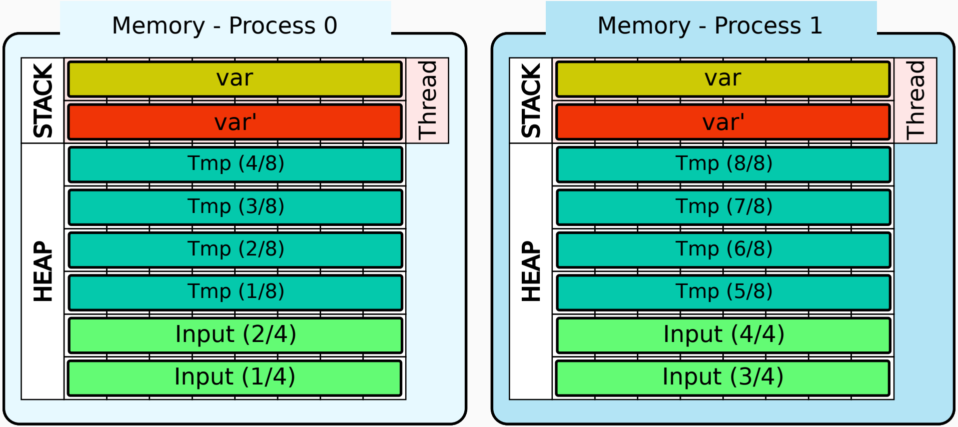


Figure 5: Distribution of initial data, focus on **runtime** data.

Improved Memory Consumption - Input Data

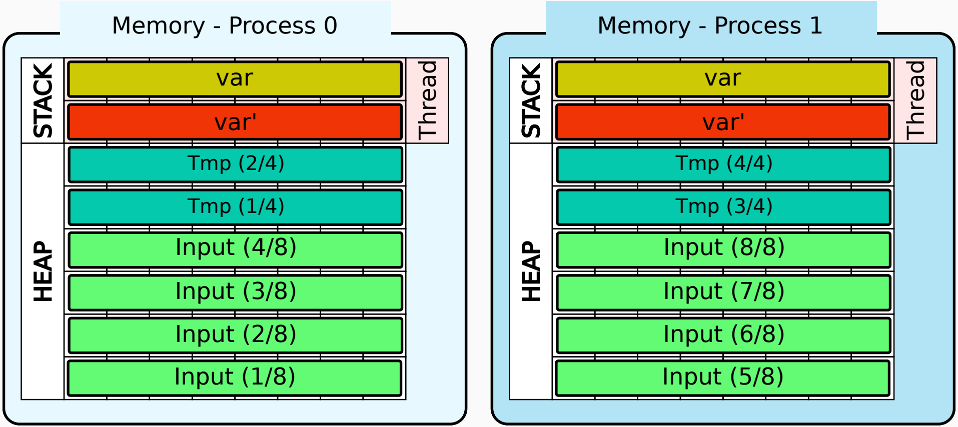


Figure 6: Distribution of initial data, focus on **input** data.

1. Add initialisation code
2. Identify and modify `malloc` calls
3. Replace OpenMP microtask
   - `@__kmpc_fork_call`
4. Modify memory accesses:
   - Inside and outside of microtask
   - Private/shared stack variables
   - Heap variables
5. Add finalisation code

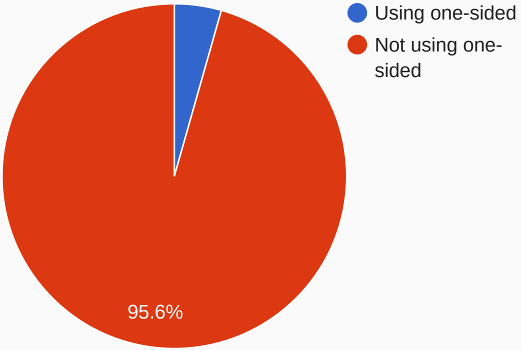


Figure 7: Usage one-sided MPI (C/C++)

IR Representation


```
%3 = tail call noalias dereferenceable_or_null(16) i8* @malloc(i64 noundef 16) #5
%4 = bitcast i32** %1 to i8**
store i8* %3, i8** %4, align 8, !tbaa !4
call void (%struct.ident_t*, i32, void (i32*, i32*, ...)*, ...) @__kmpc_fork_call(%struct.ident_t* nonnull @1, i32 1, void (i32*, i32*, ...)* bitcast (void (i32*, i32*, i32**)* @.omp_outlined. to void (i32*, i32*, ...)*), i32** nonnull %1)
```

Pass Workflow

```
RuntimeHandler r(M);
r.replace_omp_functions();
auto microtasks = find_microtasks(M);
replace_fork_calls(M, r, microtasks);
replace_memory_allocations(M, r);
replace_sequential_shared_memory_accesses(M, r);
replace_microtask_shared_memory_accesses(M, r, microtasks);
replace_parallel_for(M, r, microtasks);
replace_reductions(M, r, microtasks);
replace_criticals(M, r, microtasks);
replace_memory_deallocations(M, r);
r.adjust_netcdf_regions();
```

netCDF

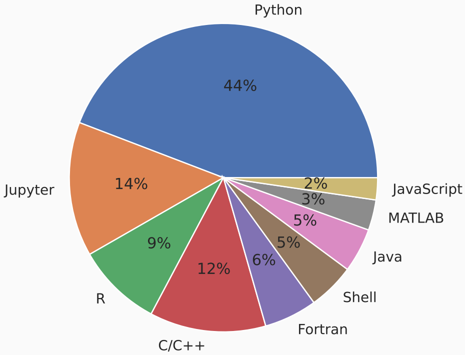


Figure 8: netCDF language distribution

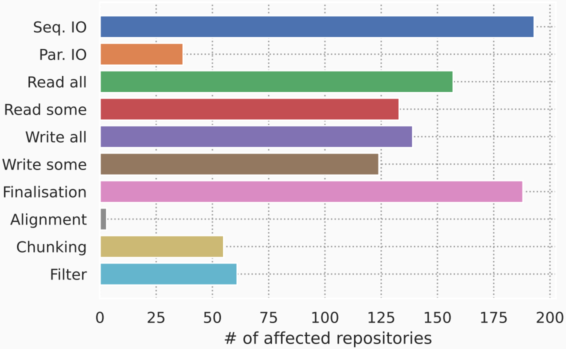


Figure 9: Used netCDF functions (C/C++)

Access via Spatial Dimensions

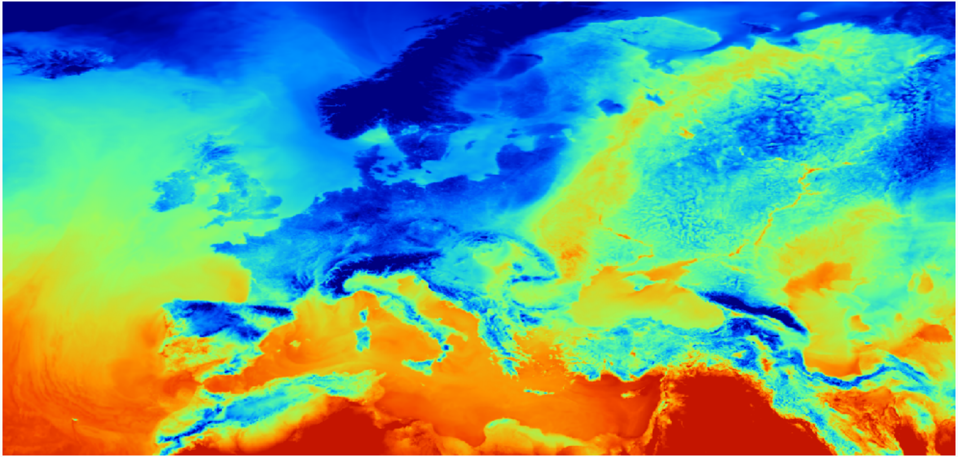


Figure 10: DWD ICON EU-nested 2m temperature from 2023-05-18-00

Access via Spatial Dimensions

- Contiguous memory layout
- Chunked data:
  - Time: slow unlimited netCDF dimension
  - Spatial dimensions: fast-varying
  - `2t:_ChunkSizes = 1, 1, 657, 1377`

$\Rightarrow$ Good read-ahead ✓

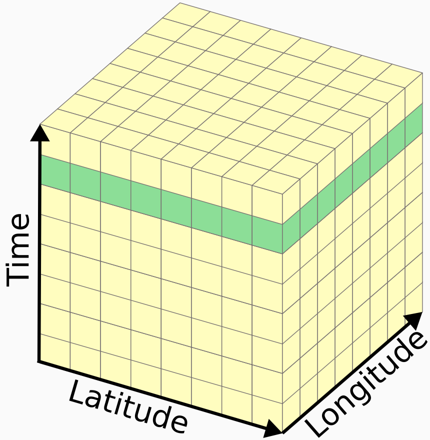


Figure 11: Convenient access pattern

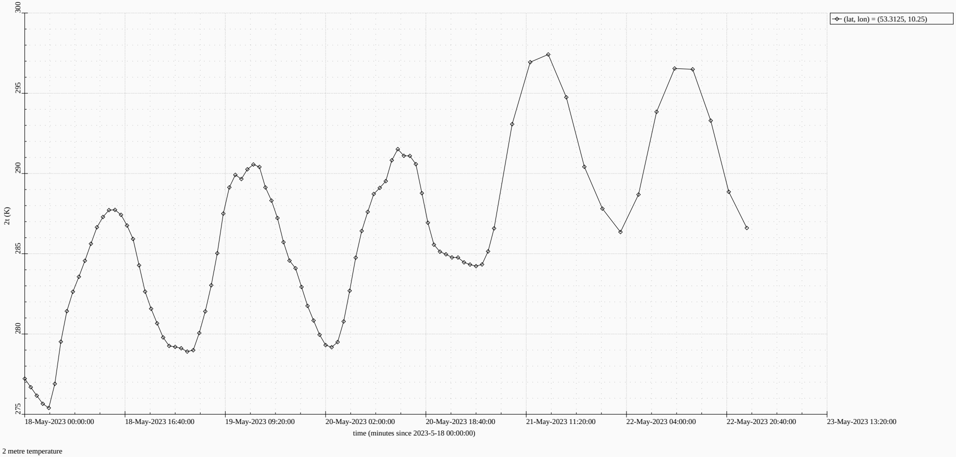


Figure 12: DWD ICON EU-nested 2m temperature time series from 2023-05-18-00 (HH)

Access via Time Dimension

- Contiguous memory layout
- Chunked data:
  - Time: slow unlimited netCDF dimension
  - Spatial dimensions: fast-varying
  - `2t:_ChunkSizes = 1, 1, 657, 1377`

⇒ ~~Good read-ahead~~

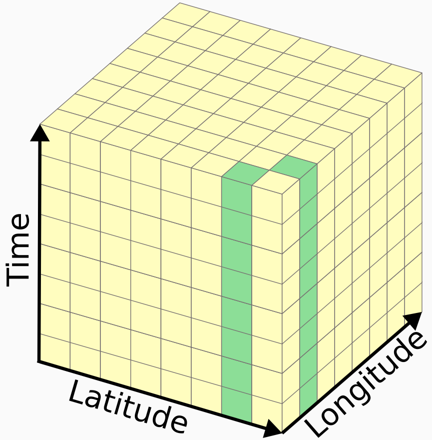


Figure 13: Inconvenient access pattern

Improved Chunking

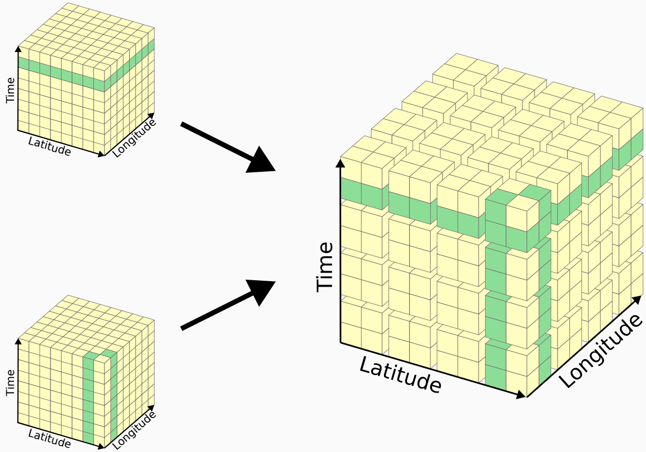


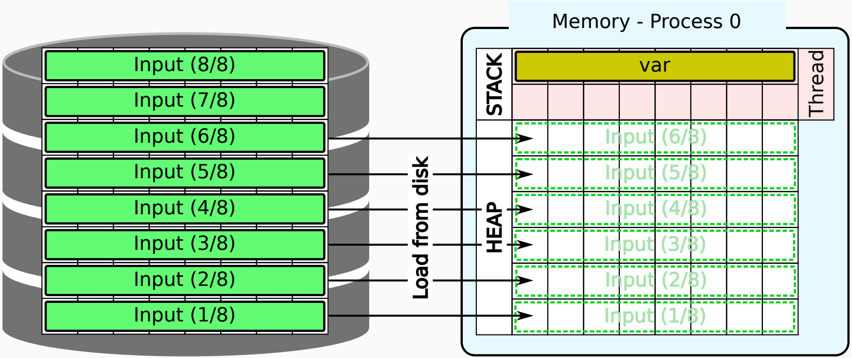
Figure 14: Combination of chunk orientations

Chunking:

- Find `nc_def_var` calls
- Add `nc_def_var_chunking`
- Add `nc_set_alignment` [BCK+15] before file initialisation

Combining parallel IO and compression makes chunking mandatory

Reading More Data



Original netCDF Workflow

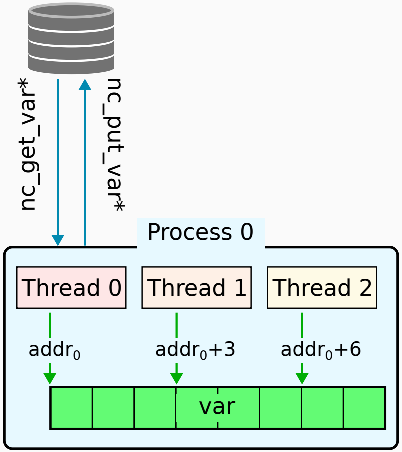


Figure 15: Access data on shared heap memory.

Modified netCDF Workflow

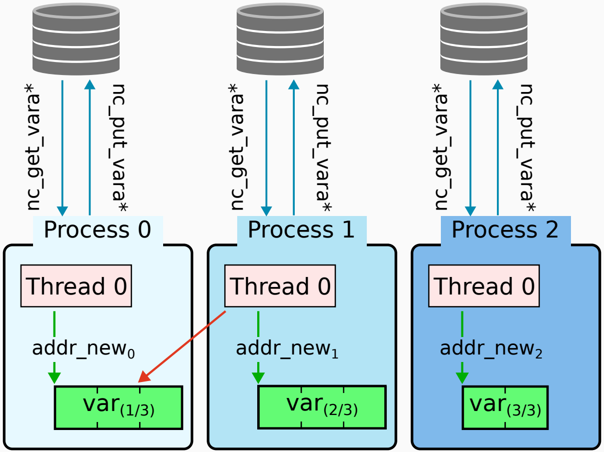


Figure 16: Access data on shared heap memory using Lustre FS.

CATO's Procedure - Parallel IO

- `nc_open` → `nc_open_par`
- `nc_create` → `nc_create_par`
- `nc_get_var*` → `nc_get_vara*`
- `nc_put_var*` → `nc_put_vara*`

Example: nc_open


```
std::optional<std::size_t> env_alignment = parse_env_size_t("CATO_NC_ALIGNMENT");
if(env_alignment.has_value()){
    alignment = env_alignment.value();
    err = nc_set_alignment(0,alignment);
}
err += nc_create_par(path, cmode, MPI_COMM_WORLD, MPI_INFO_NULL, ncidp);
check_error_code(err, "io_create_par (netCDF backend)");
```

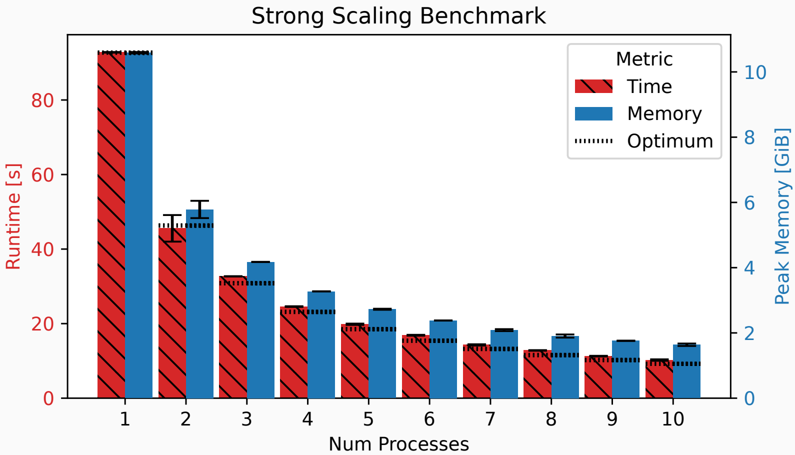
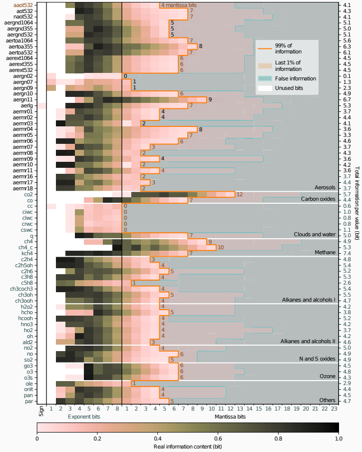


Figure 17: Benchmark using one process per node, memory peak consumption measured per node (lower is better)

Benefits of Compression

- CAMS data [IAAP+19]
- Lossless/lossy compression
- Analysis from Klöwer et al. [KRD+21, Fig. 2]



CATO’s Procedure - Filter

- Add `nc_def_var_quantize`
- Add `nc_def_var_deflate`
- Add `nc_def_var_filter`

Providing Feedback

Feedback

- Modified high-level code
  - Decompiler (RetDec [Kř23], llvm2c [sta22], LLVM-BCE [Jul22])
  - Annotated CFG (LLVis)
- Sanity Checks
  - Error checking
  - File not found
  - File not closed
- User Training
  - General introduction
  - References to official ressources
  - Tips for usage
  - References to code examples
- Optional user control via environment variables

Future Work

Memory Distribution:

- Fix bugs
- Re-introduce OpenMP
- Improve memory management
- Use MPI shared memory
- (Pattern recognition)

Parallel IO

- Feature completeness (e.g. multidimensional chunking)

Summary

- HPC is a volatile working environment
- Potential Domain scientist's struggles:
  - Confusing amount of technologies
  - Usually no trivial trying out
- Cato provides toolbox
  - Focus on natural science
  - Rapid trying out
  - 100% user space compatible
  - But: Inferior than handmade solution

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