Advanced Computation and I/O Methods for Earth-System Simulations Status update

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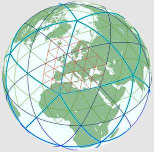
AIMES

Goals

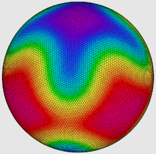
Address key issues of icosahedral earth-system models

- Enhance programmability and performance-portability
- Overcome storage limitations
- Shared benchmark for these models

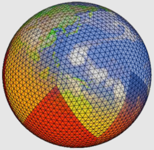
Covered models



ICON



DYNAMICO



NICAM

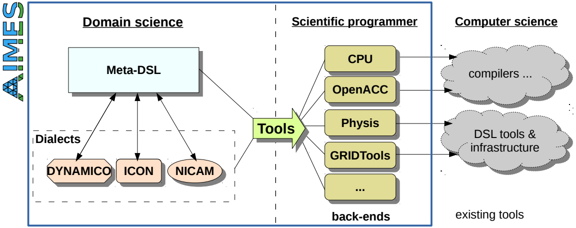
WP1: Towards Higher-Level Code Design

Recap: Goals of the WP

- Bypass shortcomings of general-purpose languages
  - Offer performance-portability
  - Enhance source repositories maintainability
  - Get rid of complexity in optimized-code development
  - Enhance code readability and scientists productivity
- Extend modelling programming language
  - Based on domain science concepts
  - Free of lower level details (e.g., architecture, memory layout)

Approach

- Foster separation of concern
  - Domain scientists develop domain logic in source code
  - Scientific programmers write hardware configurations
- Source code written with extended language
  - Closer to domain scientists logic
  - Scientists do not need to learn optimizations
  - Write code once, get performance for various configurations
- Hardware configurations define software performance
  - Written by programmers with more experience in platform
  - Comprise information on target run environment



Progress

- Achievements of the first year
  - Evaluation of GridTools for NICAM
  - HybridFortran support in ASUCA
  - Development of the model dialects and extensions
  - Implementing a basic source-to-source translation tool
  - Evaluating the DSL's impact on programmability
    Refer to: Nabeeh Jumah et al. "GGDML: Icosahedral Models Language Extensions". In: Journal of Computer Science Technology Updates. Volume 4, Number 1 (June 2017)
- Achievements of the second year
  - Refinements to the language extensions
  - Implementing more features in the translation tool
    - Configurable language extensions
    - Configurable memory layout
    - Configurable parallelization
    - Configurable halo exchange
  - Experiments on the performance and performance portability

Progress of the Third Year

- Achievements of the third year
  - Developing new test application as proxy application
    - Shallow water equations
    - Structured grid
  - Implementing more features in the translation tool to aid dev.
    - User-configuration of selected optimizations
      e.g. kernel merging to enable memory re-use
    - Configurable loop interchange and blocking
    - Supporting user-guided domain decomposition
    - Annotating kernels for Likwid instrumentation
    - Automatic generation of code to handle halo dirty regions
  - More experiments on performance (scaling, optimizations)
  - Exploring another architecture (NEC Aurora vector engine)
  - Developing a prototype for GASPI (to be evaluated)

GGDML Code Example

```
foreach c in grid
{
  float df=(f_F[c.east_edge()]-f_F[c.west_edge()])/dx;
  float dg=(f_G[c.north_edge()]-f_G[c.south_edge()])/dy;
  f_HT[c]=df+dg;
}
```

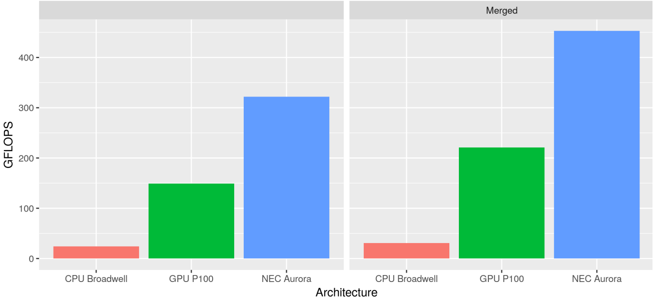
A sample generated C code for OpenMP + MPI

```
    ...handle domain decomposition and halo mangagement
  for (size_t blk_start = (0); ... blocking
    size_t blk_end = ...
#pragma omp parallel for
    for (size_t YD_index = 0; YD_index < local_Y_Cregion;
        YD_index++) {
#pragma omp simd
      for (size_t XD_index = blk_start; XD_index < blk_end;
          XD_index++) {
        float df = (f_F[YD_index][XD_index +1] -
                    f_F[YD_index][XD_index]) /dx;
        float dg = (f_G[YD_index +1][XD_index] -
                    f_G[YD_index][XD_index]) /dy;
        f_HT[YD_index][XD_index] = df + dg;
      }
```

Performance Evaluation

- Test application
  - Shallow water equations
  - Structured grid
- Test machines
  - Intel(R) Xeon(R) CPU E5-2695 v4 with 2.10GHz
    - Level 3 cache is 45 MB (shared among 18 cores)
  - Tesla P100 GPUs
  - NEC SX-Aurora TSUBASA vector engine
- Experiments
  - Efficiency on different architectures
  - Performance depending on kernel blocking

The Effect of Kernel Merging on Performance

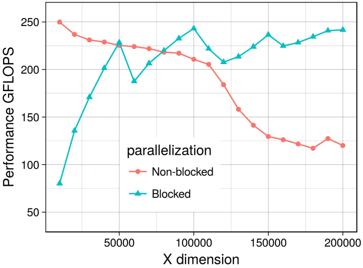


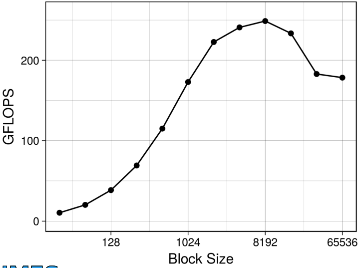
Architecture	Theoretical Memory bandwidth (GB/s)	Before merge		After merge	
		Measured memory throughput (GB/s)	GFLOPS	Measured memory throughput (GB/s)	GFLOPS
Broadwell	77	62	24	60	31
P100 GPU	500	380	149	389	221
NEC Aurora	1,200	961	322	911	453

All cases utilize between 76 and 80% memory bandwidth

Evaluation - Blocking on P100 GPUs

- Performance drop is steep around grid width of 130K as a result of the cache size
- Blocking stabilizes performance over wider grids (grid width >80K)
- Blocking harms performance for smaller grids
- The DSL can emit both





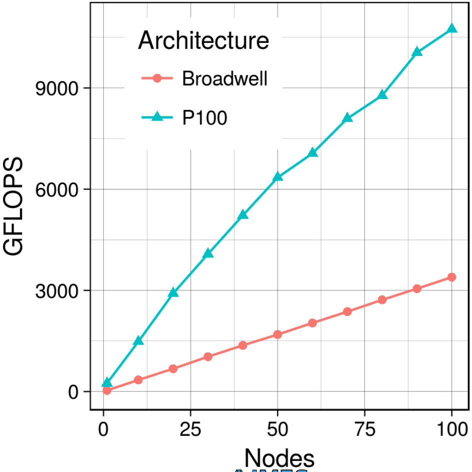
Evaluation - Vectorization and Memory Layout

- Investigation of vectorization and memory layout alternatives
- Tested three cases
  - Scattered elements: distant elements
  - Constant short distance: 4 bytes between consecutive elements
  - Contiguous (unit-stride) array
- We show impact of matching memory layout and access on
  - Vector unit and instructions utilization
  - Memory bandwidth utilization efficiency
- Allowed to simulate AoS performance

Architecture	GFLOPS		
	Scattered	Short distance	Contiguous
Broadwell	3	13	25
NEC Aurora	80	161	322

Evaluation - Scalability

- Investigation of scalability on 1,10,20..100 nodes
- Tested on Broadwell and P100 GPUs



Outlook Until the End of AIMES

- Investigate using GASPI as alternative for communication
  - Performance and other considerations
  - Differences to MPI
- Investigate semi-structured grids (again from Y1)
  - Prepare necessary configurations
  - Investigate halo exchange optimizations
  - Investigate vectorization considerations
  - Compare to structured grids
- Make the tool available on GitHub
- Provide tool for brute-force optimization exploration

Massive I/O

Recap: Goals of the WP2

- Optimization of I/O middleware for icosahedral data
  - Throughput, metadata handling
- Design of domain-specific compression (ratio $> 10 : 1$)
  - Investigate metrics allowing to define accuracy per variable
  - Design user-interfaces for specifying accuracy
  - Develop a methodology for identifying the required accuracy
  - Implement compression schemes exploiting this knowledge

Progress

- Achievements of the first year
  - C-API Design of scientific compression interface library (SCIL)
    - Quantities
    - Tools
    - Compression chain
  - Evaluation on synthetic data
  - Evaluation on scientific data (cloud model ECHAM)
- Progress in the second year
  - Survey of file formats
  - Refactoring (Project structure, quantities)
  - New tool: Pattern creator
  - HDF5 compression plug-in
  - Evaluation on synthetic data patterns
  - Evaluation on scientific data (hurricane model Isabel)

Recent Progress in Year Three

- Evaluating compression ratios/performance with NICAM files
- Integration of SCIL into NICAM
- Improved compatibility on various layers and tools
- Alternative specification of compression characteristics (in an external file)
- Investigated incremental compression algorithm
- Explored science case to identify tolerable precision loss

Configuration File for the Quantities

The file in the env. var. NETCDF_SCIL_HINTS_FILE is read by NetCDF and applied to the respective variables:

```
Variable1:
 relative_tolerance_percent=1

Variable2:        # Developer comment1
 relative_tolerance_percent=1
 relative_err_finest_abs_tolerance=1
 absolute_tolerance=1
 significant_digits=1
 significant_bits=1
 lossless_data_range_up_to=1
 lossless_data_range_from=1
 fill_value=4711
 comp_speed=0.5*MiB
 decomp_speed=1*NetworkSpeed
 force_compression_methods=abstol,lz4
```

Investigate Tolerable Error

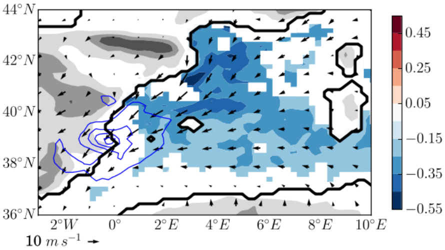
- Under noise mimicking compression, reproduce conclusions of Berthou et al. 2016[1]
  - Mediterranean region (Spain, France)
  - Evaluates how wind, through its action on the ocean, impacts (with some delay) heavy precipitation
  - Compares outputs from two simulations (CPL and SMO) and subjects the difference to tests of statistical significance
    Student t test; 97.5% probability of rejecting a zero difference
  - Analyzed fields: wind, rain (convective and non-convective), humidity, sea-surface temperature (SST)

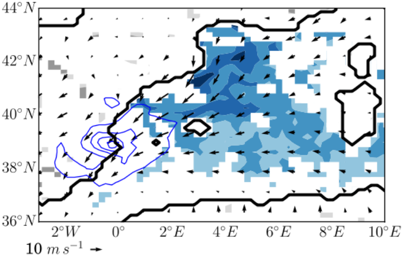
[1] DOI 10.1007/s00382-016-3153-0

Approach

1. Reproduce published results (Find data/scripts used in paper)
2. Apply statistical model for noise induced by lossy compression
   - Use Gaussian white noise
3. Redo the analysis, check if the conclusions are still supported
4. Increase levels of noise to input data (= model output)
   - One field at a time; then together

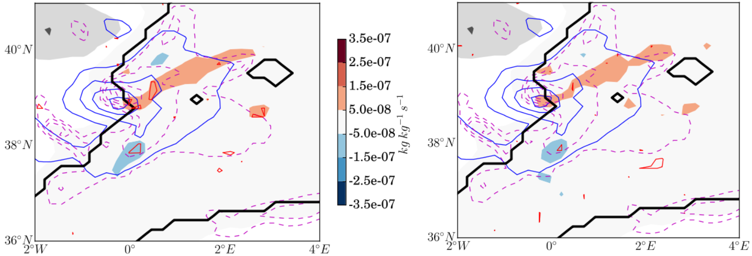
Compression Error Propagation: SST





- Blue shade: conditional mean SST difference between CPL and SMO simulations where statistical test is passed
- Adding noise affects little the overall pattern, but makes it harder to pass statistical test (more white holes in the blue)
- Conclusions unchanged even with quite large noise on SST (0.2°K), probably due to averaging several events

Compression Error Propagation: Wind



- Blue/orange shade = conditional mean difference between CPL and SMO of moisture flux divergence
  Statistical test is passed inside red contours
- Noise makes it harder to pass statistical test
- Despite noise added to wind, moisture flux divergence still OK
- Noise impact expected to worsen at higher resolution
- Projects like CORDEX2 advocate for compression methods that control noise spectrum (which is part of AIMES)

Outlook Until the End of AIMES

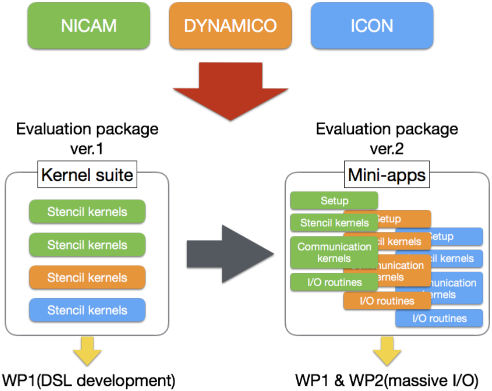
- Full application I/O benchmark with NICAM (& SCIL)
- Pushing HDF5-plugin for SCIL to HDF5 group
- Wrap-up of the documentation

We'll try to further work with students

- Integration of alternative lossy compression algorithms
- Machine learning of
  - Performance, expected ratio for data
  - Best compression algorithms

WP 3: Evaluation

- Providing benchmark packages from icosahedral weather/climate models
- Evaluating the DSL and domain-specific I/O advancements



Achievements in Year Three

- ICON kernels
  - Selection, Extraction
- ICON-like mini application
  - Written with GGDML
  - C is the host language
- Implemented NetCDF I/O support within this mini app
  - GGDML kernels support I/O
- ICON-like application integration within benchmark

Outlook Until the End of AIMES

- Integration tests
  - DSL
  - I/O
  - Compression
- Update the already published benchmark suite
  - Testcode for GGDML
  - I/O benchmarking results

Summary

- AIMES covers programmability issues on the high-level
  - DSL-extensions enrich existing languages
  - Fosters separation of concerns, improves performance portability
  - A testbed application with different kernels has been developed
  - The translation tool now supports own optimizations
  - Multi-core, GPUs, vector supported for the testcodes
- AIMES addresses domain-specific lossy compression
  - (Help) scientists to define the variable accuracy
  - Exploit this knowledge in the compression scheme
  - Novel schemes compete with existing algorithms

Backup

Backup

Differences among three icosahedral atmospheric models

- Horizontal grid system
  - NICAM: co-located, semi-structured
  - DYNAMICO: staggered, semi-structured
  - ICON: staggered, unstructured

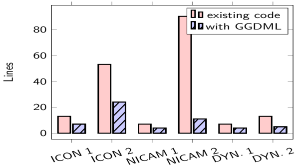
  - semi-structured means... "structured for stencil operation, unstructured for communication topology"

GGDML Impact on the Source Code

The DSL reduces development and maintenance effort

- LOC statistics

Model, kernel	lines (LOC) before DSL	lines (LOC) with DSL	words before DSL	words with DSL	characters before DSL	characters with DSL
ICON 1	13	7	238	174	317	258
ICON 2	53	24	163	83	2002	916
NICAM 1	7	4	40	27	76	86
NICAM 2	90	11	344	53	1487	363
DYNAMICO 1	7	4	96	73	137	150
DYNAMICO 2	13	5	30	20	402	218
total	183	55	911	430	4421	1991
relative size with dsl	30%		47%		45%	



- Predicting saving applying the DSL to 300k code of ICON
  - 100k infrastructure (does not change with the DSL)
  - Remaining code reduced according to our test kernels
  - COCOMO estimations

Software project	Version	Effort Applied	Dev. Time (months)	People require	dev. costs (M€)
Semi-detached		2462	38.5	64	12.3
	DSL	1133	29.3	39	5.7
Organic		1295	38.1	34	6.5
	DSL	625	28.9	22	3.1

Partners and Expertise

Funded partners

- Thomas Ludwig (Universität Hamburg)
  I/O middleware, compression, ICON DSL
- Thomas Dubos (Institut Pierre Simon Laplace)
  Application I/O servers, compression, DYNAMICO
- Naoya Maruyama (RIKEN)
  DSL (Physis), GPUs, NICAM
- Takayuki Aoki (Tokio Institute of Technology)
  DSL (HybridFortran), language extension, peta-scale apps

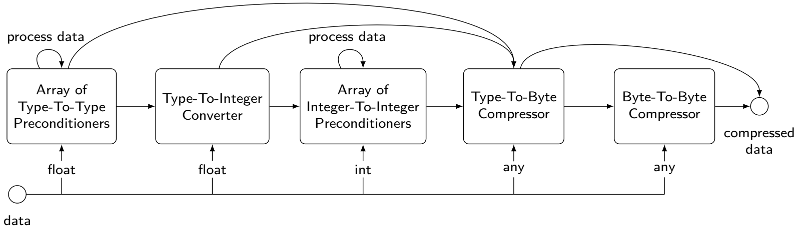
Cooperation Partners

- DKRZ *(I/O, DSL)*
- DWD *(ICON, DSL, I/O)*
- University of Exeter *(Math. aspects in the DSL)*
- CSCS *(GPU/ICON, GRIDTool, compression)*
- Intel *(DSL-backend optimization for XeonPhi, CPU)*
- NVIDIA *(DSL-backend optimization for GPU)*
- The HDF Group *(I/O, unstructured data, compression)*
- NCAR (MPAS developers, another icosahedral model)
- Bull
- Cray

Information exchange, participate in workshops, [hardware access]

Appendix. WP2: Architecture of SCIL

- Contains tools to
  - Create random patterns, compress/decompress, add noise, plot
- HDF5 and NetCDF4 integration; tools support NetCDF3, CSV
- Library with
  - Automatic algorithm selection (under development)
  - Flexible compression chain:



WP2: Supported Quantities

Accuracy quantities:

absolute tolerance: compressed can become true value ± absolute tolerance

relative tolerance: percentage the compressed value can deviate from true value

relative error finest tolerance: value definining the absolute tolerable error for relative compression for values around 0

significant digits: number of significant decimal digits

significant bits: number of significant decimals in bits

Performance quantities:

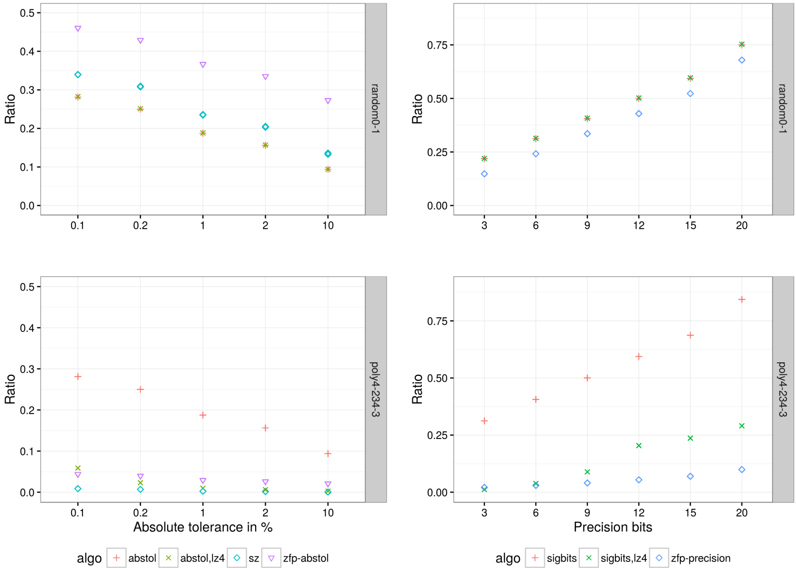
compression speed: in MiB or GiB, or relative to network or storage speed

decompression speed: in MiB or GiB, or relative to network or storage speed

Supplementary quantities:

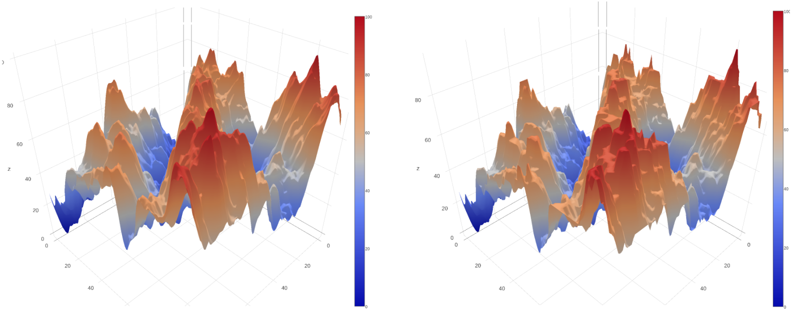
fill value: a value that scientists use to mark special data point

WP2: Synthetic Patterns



WP2: Example Synthetic Data

Simplex (options 206, 2D: 100x100 points)



Right picture compressed with Sigbits 3bits (ratio 11.3:1)

WP2: Analyzing Performance of Lossy Compression

Data

- Single precision (1+8+23 bits)
- Synthetic, generated by SCIL's pattern lib.
  - e.g., Random, Steps, Sinus, Simplex
- Data of the variables created by ECHAM (123 vars), Isabel

Experiments

- Single thread, 10 repeats
- Lossless (memcopy and lz4)
- Lossy compression with significant bits (zfp, sigbits, sigbits+lz4)
- Lossy compression with absolute tolerance (zfp, sz, abstol, abstol+lz4)
  - Tolerance: 10%, 2%, 1%, 0.2%, 0.1% of the data maximum value

WP2: Comparing Algorithms for the Scientific Files

	Algorithm	Ratio	Compr. MiB/s	Decomp. MiB/s
ECHAM	abstol	0.190	260	456
	abstol,lz4	0.062	196	400
	sz	0.078	81	169
	zfp-abstol	0.239	185	301
Isabel	abstol	0.190	352	403
	abstol,lz4	0.029	279	356
	sz	0.016	70	187
	zfp-abstol	0.039	239	428
Random	abstol	0.190	365	382
	abstol,lz4	0.194	356	382
	sz	0.242	54	125
	zfp-abstol	0.355	145	241

(a) 1% absolute tolerance

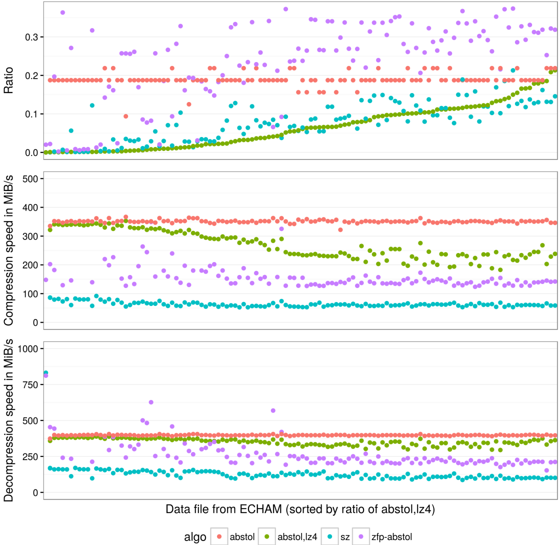
	Algorithm	Ratio	Compr. MiB/s	Decomp. MiB/s
ECHAM	sigbits	0.448	462	615
	sigbits,lz4	0.228	227	479
	zfp-precision	0.299	155	252
Isabel	sigbits	0.467	301	506
	sigbits,lz4	0.329	197	366
	zfp-precision	0.202	133	281
Random	sigbits	0.346	358	511
	sigbits,lz4	0.348	346	459
	zfp-precision	0.252	151	251

(b) 9 bits precision

Table: Harmonic mean compression of scientific data

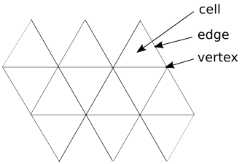
WP2: Results for Absolute Tolerance of ECHAM

Comparing algorithms using an absolute tolerance of 1% of the maximum value

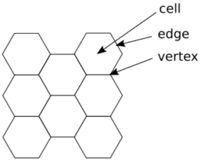


DSL Development

- Co-design with scientists to develop DSL constructs
  - Current version represents several iterations
  - GGDML: *General grid definition and manipulation language*
  - Grid definition
  - Grid-bound variable declaration
  - Grid-bound variable access/update
  - Stencil operations
- Hides memory locations and access details, data iteration
- Abstract higher concepts of grids, hiding connectivity details



a) Triangular grid



b) Hexagonal grid

Progress of WP3

- Achievements in the first year
  - NICAM kernels
    - Selection, Extraction
    - Performance check (on the K computer(RIKEN), Mistral(DKRZ))
  - DYNAMICO and ICON kernels
    - Selection
  - tools for damping the reference data
- Progress of the second year
  - Packaging IcoAtmosBenchmark v.1
  - NICAM kernels
    - Documents
    - Implementation by GridTools
  - DYNAMICO kernels
    - Extraction, Performance check, Documents