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

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Motivation

- Several groups work on icosahedral-grid based climate/weather models
- Obstacles for Exascale simulations - but also on small scale:
  - Code is very complex and difficult to refactor
  - Climate prediction creates huge data volumes

Limitations of general-purpose programming languages

- Semantics and syntax restrict programmers productivity
- Performance is hardly portable between architectures

Existing Domain-Specific Languages

- May create optimized code for different architectures
- Technical languages with limited relation to scientific domain
- Typically require language-specific paradigm shift for scientists
- Unclear future of the framework/tool

Existing scientific file formats

- Metadata for icosahedral data is not standardized
- Difficult to achieve good performance
- Pre-defined compression schemes achieve suboptimal ratio

Goals

Address issues of icosahedral earth-system models

- Enhance programmability and performance-portability
- Overcome storage limitations
- Provide a common benchmark for icosahedral models

Collaboration

Funded partners

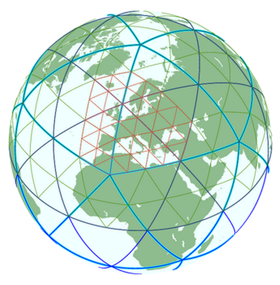
- Thomas Ludwig (Universität Hamburg)
- Thomas Dubos (Institut Pierre Simon Laplace)
- Naoya Maruyama (RIKEN)
- Takayuki Aoki (Tokio Institute of Technology)

Collaboration partners

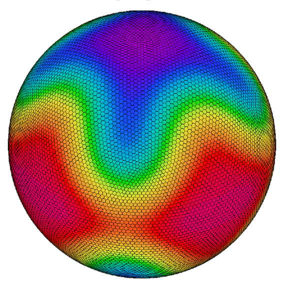
- DKRZ *(I/O, DSL)*
- DWD *(ICON, DSL, I/O)*
- University of Exeter *(Mathematic aspects in the DSL)*
- CSCS *(GPU/ICON, GRIDTool, compression)*
- Intel *(DSL-backend optimization for XeonPhi, CPU)*
- NVIDIA *(DSL-backend optimization for GPU)*
- The HDF Group *(I/O, unstructured data, compr.)*
- NCAR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

Information exchange, participation in workshops...

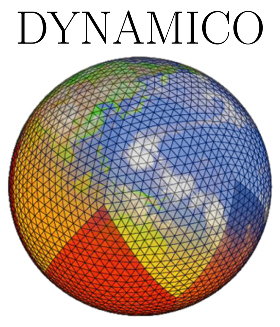
Models



ICON



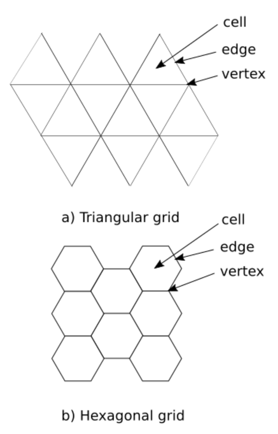
DYNAMICO



NICAM

GGDML Domain-Specific Language

- GGDML: General Grid Definition and Manipulation Language
- Abstracted scientific-domain based constructs for:
  - Data types reflecting "grid" concepts
  - Variable Declaration & allocation on cells, edges and vertices
  - Iterators to traverse and update variables
  - Named neighbours in (triangular/hexagonal) grids
- Developed in co-design with domain scientists



Fortran code (dynamico) and GGDML version

```
DO l=ll_begin,ll_end
!DIR$ SIMD
  DO ij=ij_begin,ij_end
   berni(ij,l) = .5*(geopot(ij,l)+geopot(ij,l+1)) + 1/(4*Ai(ij)) *
       (le(ij+u_right)*de(ij+u_right)*u(ij+u_right,l)**2 &
       +le(ij+u_rup)  *de(ij+u_rup)  *u(ij+u_rup,l)**2   &
       +le(ij+u_lup)  *de(ij+u_lup)  *u(ij+u_lup,l)**2   &
       +le(ij+u_left) *de(ij+u_left) *u(ij+u_left,l)**2  &
       +le(ij+u_ldown)*de(ij+u_ldown)*u(ij+u_ldown,l)**2 &
       +le(ij+u_rdown)*de(ij+u_rdown)*u(ij+u_rdown,l)**2 )
  ENDDO
ENDDO
```

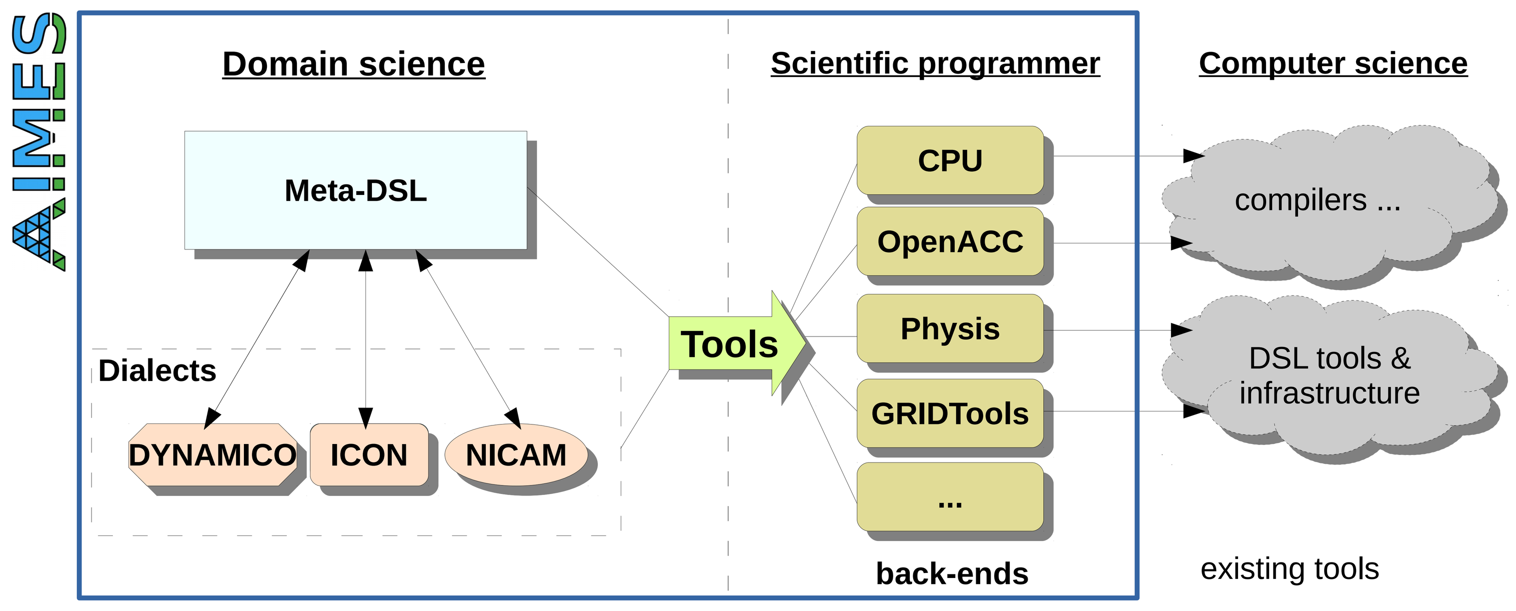
GGDML version of the code above

```
FOREACH cell IN grid
 berni(cell) = .5*(geopot(cell)+geopot(cell%above)) + 1/(4*Ai(cell%ij)) *
  REDUCE(+, N={1..6}
    le(cell%neighbour(N)%ij)*de(cell%neighbour(N)%ij)*u(cell%neighbour(N))**2)
END FOREACH
```

Scientific Work Packages: Objectives and Tasks

WP 1: Towards higher-level code design

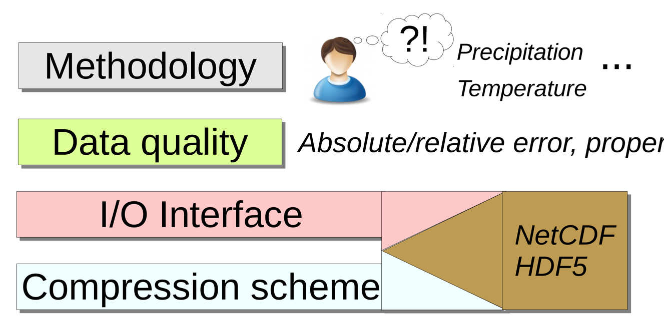
- Foster separation of concerns: Domain scientists, scientific programmer and computer scientists
  - High level of abstraction, reflects domain science concepts
  - Independence of hardware-specific features, e.g. memory-layout
  - Convertible into existing languages and DSLs



- 1.1-1.3 Develop and reformulate key parts of models into DSL-dialects
- 1.4 Design common DSL concepts for icosahedral models
- 1.5 Develop source-to-source translation tool and mappings

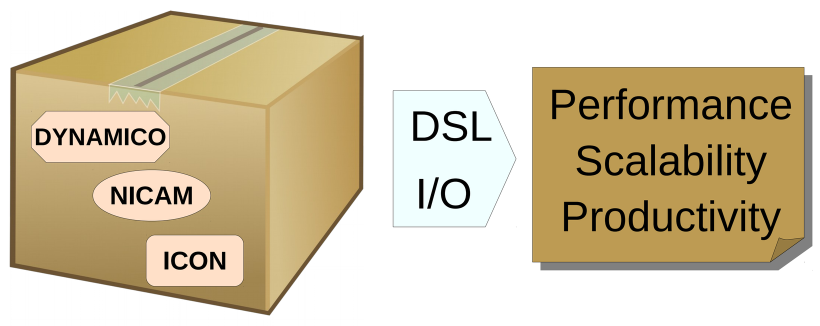
WP 2: Massive I/O

- 2.1 Optimize file formats for icosahedral data
- 2.2 Data reduction concepts
- 2.3 API for user-defined variable accuracy
- 2.4 Identifying required variable accuracy
- 2.5 Lossy compression



WP 3: Evaluation

- 3.1 Selection of representative test cases
- 3.2 Extraction of simple kernels
- 3.3 Common benchmark package/mini-IGCMs[1]
- 3.4 Benefit of the DSL for kernels/mini-IGCMs
- 3.5 Estimating benefit for full-featured models
- 3.6 I/O advances for full models



DSL Tools

Source-to-source translation

- Translates GGDML code into
  - architecture-optimized code OR intermediate language
- Light-weight easily maintainable translation tool, shipped with code
  - Integratable into Build-Systems
  - Offers a configurable translation procedure
  - Initial prototype with limited functionality is complete

Compilation profiling

- Learns optimal compilation options for each repository file
- Minimizes time of repository builds while keeping code performance

Initial results (single node)

- Performance and compilation procedures have been explored
  - Different compilers (Intel, GCC, CLang)
  - Different compilation options
  - Different memory layouts

- Testsystem
  - Intel i7-6700 @3.4 GHz
  - Skylake, 4 cores
- Optimization levels
  - O0 – O3
  - Profile guided optimiz.
- Memory layouts
  - 2D Hilbert filling curve with vertical dimension
  - 3D Hilbert filling curve with indirect addressing
  - 1D transformation of 3D Euclidean space
  - 3D Euclidean space
- Intel 1D is fastest
- GCC 1D/3D with PGO next
- Indirect indexing slowest
- GCC good PGO benefit (auto vectorization)
- CLANG PGO no benefit
- Hyperthreading benefit
  - But balance work on cores

Compression

- Development of Scientific Compression Library `https://github.com/JulianKunkel/scil`
- Users define the required accuracy
  - In terms of relative/absolute/precision ...
  - In terms of required performance
  - The library picks a fitting algorithm
- Integration into HDF5 / NetCDF4

Extending NICAM with a high-levle framework

- GridTools
  - C++ template framework for weather and climate models
  - Architecture-independent programming interface for performance and portability
- Evaluating GridTools as a programming framework for NICAM
- Successfully ported representative NICAM stencil kernels with comparable performance as hand-tuned implementations

Acknowledgement

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`https://wr.informatik.uni-hamburg.de/research/projects/aimes/start`