Empowering Scientists with Domain Specific Languages

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Outline

Developing Scientific Applications

Runtime perspective

- Performance demanding
- Earth system modelling is an example
  - More precise forecasts ⇒ higher resolution grids
  - Ensemble computation
- Should exploit available compute resources
- HPC landscape increasingly inhomogene

Development view

- Productivity should be the goal
- Software readability/maintainability is a challenge
  - Continuous code changes due to experimental character
  - Branches to optimize code for different systems
- Software engineering concepts rarely used (agile development)

Readability: Semantics of Computation

Example

- Goal: multiplication of two matrices
- Scientists perspective: $C = A \cdot B$

Programming

- In Matlab: $C = A * B$ alternatively $C = mtimes(A, B)$
- In Mathematica: $C = A.B$
- In R: C = A %*% B
- In Fortran: $C = matmul(A, B)$
- In NumPy: $C = np.matmul(A, B)$
- Optimized math library – BLAS for C/Fortran:
  $DGEMM(TransA, TransB, M, N, K, ALPHA, A, LDA, B, LDB, BETA, C, LDC)$

Code Optimizations Lead to Diversification

BLAS levels

- BLAS1 Vector operations
- BLAS2 Matrix-Vector operations
- BLAS3 Matrix-Matrix operations

Reason for additional levels

- Reduce coding effort
- Efficient reuse of cache ⇒ minimize memory transfers

Outlook

- Optimize calling multiple BLAS3 routines? BLAS4+?
- Compile-time or runtime system needed !

Stencil Computation

Usage

- Finite difference methods in climate/weather
- Numerical methods (explicit or implicit)
- Potentially low arithmetic density, needs cache reuse!

Cache Reuse with Stencils

- Example with three stencils:

```
for each timestep:
  applyStencil(S1, in:{varA, varB}, out:varC)
  applyStencil(S2, in:{varA, varC}, out:varD)
  applyStencil(S3, in:{varB, varD}, out:varA)
```

- Mandatory to optimize across stencils
- Machine dependent optimizations, autotuning necessary

Capabilities of Compilers

Limitations of optimization strategies

- E.g., Vectorization, loop unrolling, interprocedural analysis
- Needs information about execution to perform optimization
- Must follow the semantics of the (general purpose) language
- Based on pattern matching, often full potential is not used
- **Not available:** memory layout adaption, cache management

Optimization time

- Traditionally: at compile time (also true for C++ templates)
- Profile guided optimization provides some runtime information
- Just-in-time compilers (runtime, may create special versions)
- Runtime: Lazy execution by library compilers (Big Data tools)

Runtime: Lazy execution by Library Compilers

Concept

- GPL is used to setup control flow
  - GPL compiler won't optimize performance critical code-regions
- Library provides functions to register and start computation
- Library generates (optimal) architecture-specific code
  - Exploiting semantics of the library
  - All information needed to create code is available in memory

Example

```
registerStencil(S1, in:{varA, varB}, out:varC)
registerStencil(S2, in:{varA, varC}, out:varD)
registerStencil(S3, in:{varB, varD}, out:varA)
executeStencils(timesteps)
```

Development Approaches

- Manual optimization of source code:
  - Adjust code to be easily consumable/optimizable by compilers
  - Reduces code readability, many branches
  - Complicates maintainability
- Libraries:
  - Provide optimized codes usable across applications
  - Address multiple target architectures
  - Machine-dependent solutions
  - Optimization across library calls often not possible
- Just-in-time and runtime compilers:
  - Complex to develop und understand
  - Compile overhead (to machine representation) at runtime
- Domain-specific languages:
  - High-level semantics of application users possible
  - Potentially code-preparation at compile time or runtime

Domain-Specific Languages

Domain-specific language (DSL)

Language assisting to describe (solutions for) problems within a certain domain

Technical vs. domain-oriented DSLs

- Technical DSL helps to formulate technical requirements
  - Instructions for the “compiler“ to perform certain optimizations
  - Need further effort and technical knowledge from scientists.
  - Example: OpenMP, OpenACC, ...
- Domain-oriented DSL
  - Serves the scientists productivity (expressive, ease of use)
  - At best: write code as you describe the problem in the domain
  - System can exploit the semantics to optimize on different levels
  - Generates (optimized) code for a specific architecture
  - Acceptance from scientists is crucial

Domain-Specific Languages: Classification

Standalone vs. language extensions

- Standalone DSLs
  - Enables paradigm shift to, e.g., declarative programming
  - Complete language, requires rewrite of existing code
- Language extensions
  - Built on an existing general-purpose language
  - Introduces constructs not understood by the GPL compiler:
    - Needs an own compiler, preprocessor, or
    - Source-to-source code translation (DSL $\Rightarrow$ GPL code)
  - May support incremental porting of code

Domain-Specific Languages

ATMOL

- A domain-specific language
- Used for atmospheric modeling
- Declarative high-level constructs
  - Declare independent variables
  - Declare dependent variables
    - Data types
    - Lower/Upper bounds
    - Units
  - Including scalars and fields
  - Declare new PDE operators
  - PDEs are defined with arithmetic expressions
  - Boundary conditions support via conditional expressions
- Translated into efficient numerical codes

ATMOL code examples

```
% Declare spatial and time dimensions:
space (x(i),y(j),z(k)) time t.

% Declare grid size variables n, m, and l:
n :: integer(1..infinity); m :: integer(1..infinity); l :: integer(2..infinity).

% For convenience, define macros for two grid domains spanning (i,j,k):
atmosphere := i=1..n by j=1..m by k=1..l; surface := i=1..n by j=1..m.

% Set coordinate system for symbolic derivation with chain-rule:
coordinates := [x, y]; coefficients := [h x, h y].

% Declare the model fields:
u::float dim "m/s" field (x(half),y(grid),z(grid)) on atmosphere.
v::float dim "m/s" field (x(grid),y(half),z(grid)) on atmosphere.
u_aux::float dim "Pa m/s" field (x(half),y(grid),z(half)) on atmosphere.
v_aux::float dim "Pa m/s" field (x(grid),y(half),z(half)) on atmosphere.
p::float(0..107000) dim "Pa" field(x(grid),y(grid),z(grid))
        monotonic k(+) on atmosphere.
p_s_t::float dim "Pa/s" field (x(grid),y(grid)) on surface.

% Define macro for the horizontal wind velocity vector components:
V := [u_aux, v_aux].

% Equations:
p_s_t = -int(nabla .* V, z=1..l).
V = [u, v] * d p/d z.
```

PATUS DSL

- A code generation and auto-tuning framework
- Domain: Stencil computations
  - Stencil specifications embedded in a C-like DSL
- Optimization strategy
  - A special DSL is provided to specify a strategy
  - Parametrized for autotuning
- Architecture-specific optimized C code is generated

PATUS Stencil Specification Example

```
stencil uxx1
{
 domainsize = (nxb .. nxe, nyb .. nye, nzb .. nze);
 t_max = 1;

 operation (
   const float grid d1(-1..nx+2,-1..ny+2,-1..nz+2),
   float grid u1(-1..nx+2, -1..ny+2, -1..nz+2),
   const float grid xx(-1..nx+2,-1..ny+2,-1..nz+2),
   const float grid xy(-1..nx+2,-1..ny+2,-1..nz+2),
   const float grid xz(-1..nx+2,-1..ny+2,-1..nz+2),
   float param dth)
  {
   float c1 = 9./8.;
   float c2 = -1./24.;

   float d = 0.25 * d1[x,y,z] + d1[x,y-1,z] +
     d1[x,y,z-1] + d1[x,y-1,z-1]);
   u1[x,y,z; t+1] = u1[x,y,z; t] + (dth / d) * (
     c1 * (
       xx[x,y,z] - xx[x-1,y, z ] +
       xy[x,y,z] - xy[x, y-1,z ] +
       xz[x,y,z] - xz[x, y, z-1]) +
     c2 * (
       xx[x+1,y, z ] - xx[x-2,y, z ] +
       xy[x, y+1,z ] - xy[x, y-2,z ] +
       xz[x, y, z+1] - xz[x, y, z-2])
  );
  }
}
```

PATUS Strategy Example

```
strategy cacheblocking (domain u, auto dim cb,
  auto int chunk)
{
  // iterate over time steps
  for t = 1 .. stencil.t_max
  {
    // iterate over subdomain
    for subdomain v(cb) in u(:; t)
      parallel schedule chunk
    {
      // calculate the stencil for each point
      // in the subdomain
      for point p in v(:; t)
        v[p; t+1] = stencil (v[p; t]);
    }
  }
}
```

STELLA DSL

- A domain-specific extended language
  - Uses template metaprogramming within C++
  - A user writes a single code
  - An operator is defined with stages
  - Python support with stencil formulation
- Code is translated at compile time for a specific architecture
  - Loops are generated for the architecture
  - A user-provided functor is used to generate the stencil code
- Multiple backends
  - Multicore CPUs with OpenMP
  - GPUs with CUDA
- A specific memory layout is used for each backend
- Automatically fuses operator stages to enhance locality

STELLA Code Example

The Laplacian operator as a stage for Horizontal Diffusion

```
// declarations
IJKRealField data;
Stencil horizontalDiffusion;

// declare stencil stage
template<typename TEnv>
struct Laplace {
  STENCIL STAGE(TEnv)

  STAGE PARAMETER(FullDomain, phi)
  STAGE PARAMETER(FullDomain, lap)

  static void Do(Context ctx, FullDomain) {
  ctx[lap::Center()] = -4.0 * ctx[phi::Center()] +
     ctx[phi::At(iplus1)] + ctx[phi::At(iminus1)] +
     ctx[phi::At(jplus1)] + ctx[phi::At(jminus1)] ;
  }
};
```

STELLA code example

Two-stage horizontal diffusion, with Laplacian and Divergence

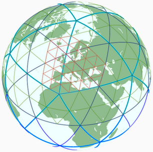
```
//define and initialize the stencil
StencilCompiler::Build(
  horizontalDiffusion,
  // define the input/output parameters,
  pack parameters(
    Param<res, cInOut>(dataOut), Param<phi, cIn)(data)
  ),
  define temporaries(
    StencilBuffer<lap, double, KRange<FullDomain,0,0> >(),
  ),
  define loops(
    define sweep<cKIncrement>(
      define stages(
        StencilStage<Laplace, IJRange<cIndented,-1,1,-1,1>,
          KRange<FullDomain,0,0> >(),
        StencilStage<Divergence, IJRange<cIndented,0,0,0,0>,
          KRange<FullDomain,0,0> >(),
      )
    )
  )
);
// execute the stencil instance
horizontalDiffusion.Apply();
```

AIMES Project

Address key issues of icosahedral earth-system models

- **Enhance programmability and performance-portability**
- Increase storage efficiency
- Provide a common benchmark for ICO models

Covered models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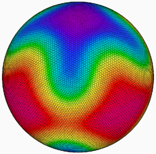
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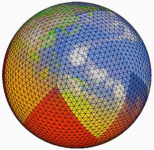
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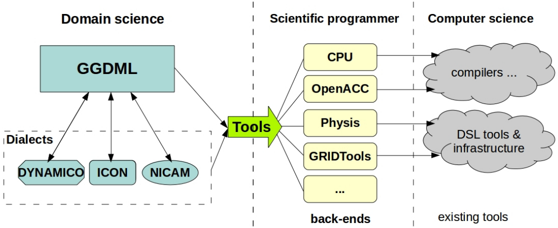
AIMES higher level coding approach

- Re-arrange model development workload
  - 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 optimization
  - 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



AIMES Approach

Approach

- We build a translation tool that is configurable
  - Language can be adjusted for the needs of the scientists
  - Processing engine should reduce repeating patterns (in GPL)
  - GGDML language example discussed with ICO* model teams
- Parses language extension of GPL code
- Can be used for a bottom up approach for simplifying code
  - Incremental adoption possible (if memory layout is unchanged
- Lightweight compiler infrastructure (self maintainable)
  - Providing cross kernel optimizations

The Laplacian operator with GGDML (as part of Fortran/C)

```
FOREACH cell IN GRID
 lap(cell) = 4*h(cell)-( REDUCE(+,N={1..4},h(cell%neighbour(N))  )
END FOREACH
```

AIMES Experiments to Show Layout Dependency

Test kernel

- Part of an icosahedral modeling testbed
- Two target architectures: CPU and GPU (unified memory)
- Parallelization: OpenACC for GPU and OpenMP for CPU
- Two memory layouts (3D vs. 1D)
- 5, 7, and 9 point stencils

Configuration

- CPU: Ivy Bridge E5-2690 v2 3.0GHz (SP: 240 GFLOP/s)
- GPU: Nvidia K80 (SP: 6 TFLOP/s)
- GPU: P100 (SP: 9-10 TFLOP/s)
- Compiler: PGI 17.5 C

AIMES Experiments

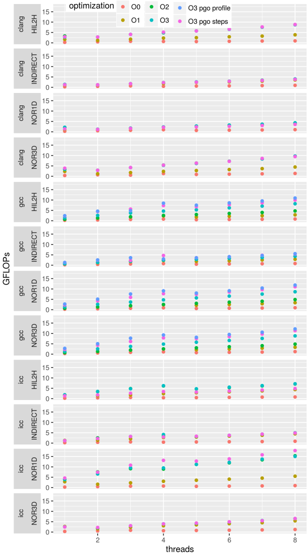
Performance

Stencil	CPU Performance (GFlops/s)		K80 GPU Performance (GFlops/s)		P100 GPU Performance (GFlops/s)	
	Normal 3D array	1D addressing	Normal 3D array	1D addressing	Normal 3D array	1D addressing
5	71	72	78	128	189	342
7	97	97	93	169	243	394
9	112	117	102	195	287	431

- Memory layout's impact on performance is high
- Caching on the GPU added ~25% performance

CPU Measurements Compiler Stuff

- Previous experiments for CPU
  - Div, Rad, Grad stencil kernels
  - Skylake CPU
- Explored opt. of mem. layout
  - 3D and 1D transformation
  - Hilbert filling curves & HEVI
  - With various compilers
    - Intel, GCC, CLang
- Best layout depends on compiler!



Summary

- Scientists should harness methods to improve readability
  - As close as possible to the domain's typical code formalization
  - Abstracting from technical details
    - Compute backend, memory layout, loops, cache mgmt
  - Supporting (semi) automatic optimization / autotuning
- Separation of concerns eases understanding/speeds up dev.
  - Scientist – scientific programmer – computer scientist
  - Abstraction from memory layout
- We are working on a generic tool to reduce code replication
  - Providing a customizable DSL suitable for any domain
  - Exploiting optimization strategies beyond compiler capabilities
- Community could define language(s) to express their problems

- Other tools relevant for atmospheric modeling:
  - BLAS-Like Library Instantiation Framework (BLIS)
  - Firedrake (PDE solver system)

Advertisement

- **Workshop Exascale I/O for Unstructured Grids (EIUG)**
- When: Monday/Tuesday 25th/26th of Sept.
- Where: Hamburg, DKRZ
- Speakers: Storage experts, domain experts
- Funding is available!
- `https://wr.informatik.uni-hamburg.de/events/2017/eiug`