FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
FACULTY OF ENGINEERING

Whole program generation for Ocean Models

ESiWACE2 VIRTUAL workshop on *Emerging Technologies for Weather and Climate Modelling*. 30.06.2020

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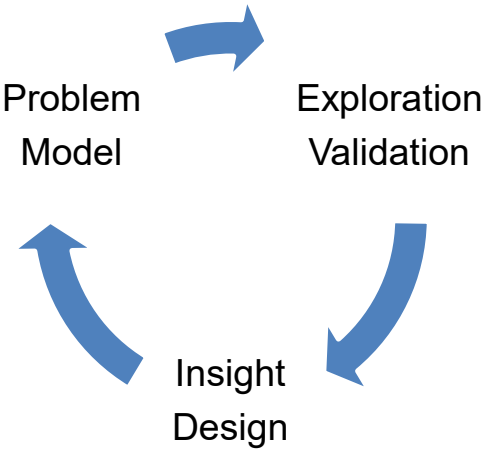
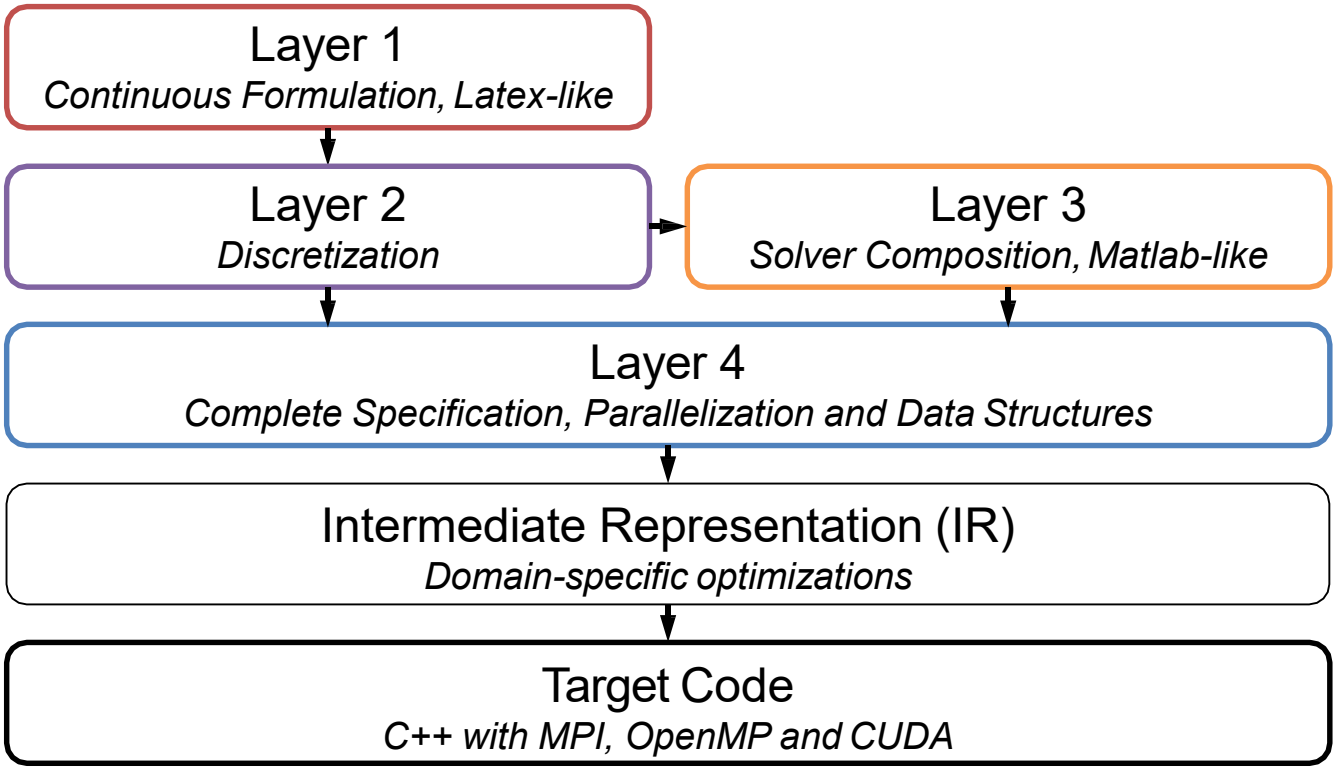
Research Vision

- **Automize the HPC software development process**
- **Increase**
  - *Performance*: by smart numerical algorithms and performance engineering
  - *Portability*: by using domain-specific compilers or code transforms to produce concrete implementations
  - *Productivity*: by working on different layers of abstract descriptions and separation of concerns

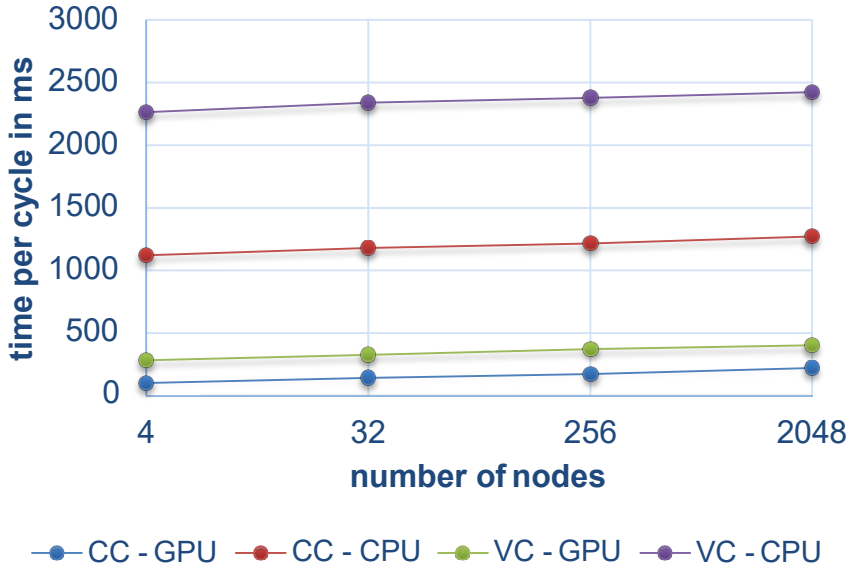


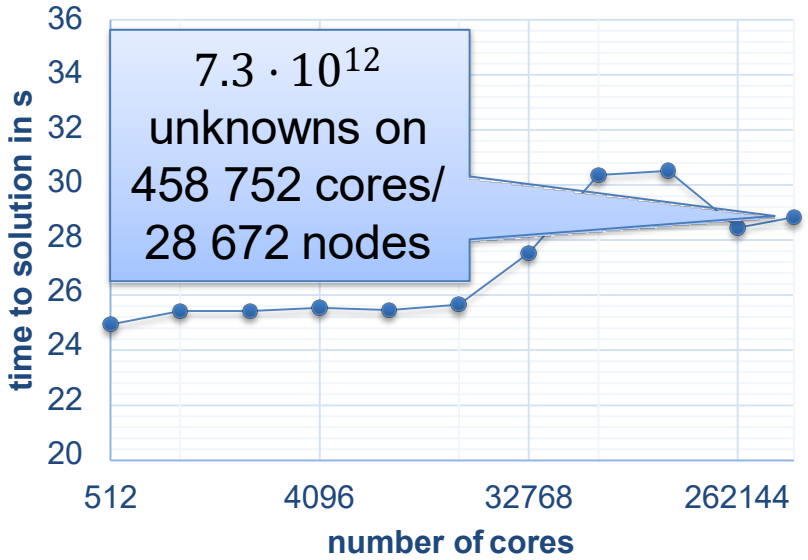
The full program generation ExaStencils approach (for geometric multigrid solvers)

Workflow (DFG SPPEXA 2013-2019, 5 PhD students)



Does it run well on supercomputers?





- Pure MPI & CUDA

- Hybrid MPI/ OpenMP

The full simulation generation ExaStencils approach (for block-structured grids and DG)

Mathematical model for the 2D Shallow Water Equations (SWE)

$$\frac{\partial \xi}{\partial t} + \nabla \cdot (\boldsymbol{U}) = 0 \tag{1}$$

$$\frac{\partial (\boldsymbol{U})}{\partial t} + \nabla \cdot ((\boldsymbol{U})(\boldsymbol{U})^T / H) + \tau_{bf} \boldsymbol{U} + f_c \boldsymbol{k} \times \boldsymbol{U} + gH \nabla \xi = \boldsymbol{F} \tag{2}$$

ξ : elevation of the free water surface

$H = h_b + \xi$: total fluid depth

h_b : bathymetric depth

$\boldsymbol{U} = (U, V)^T$: depth integrated horizontal velocity field

f_c : Coriolis parameter

$\boldsymbol{k}$: local vertical vector

g : gravitational acceleration

τ_{bf} : bottom friction coefficient

$\boldsymbol{F}$: forcing term

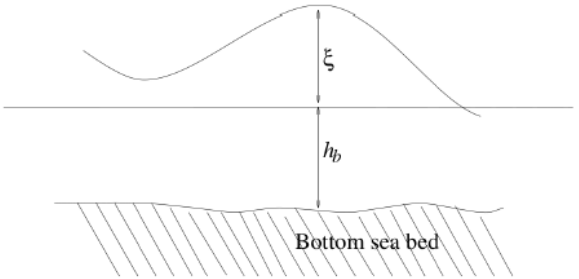
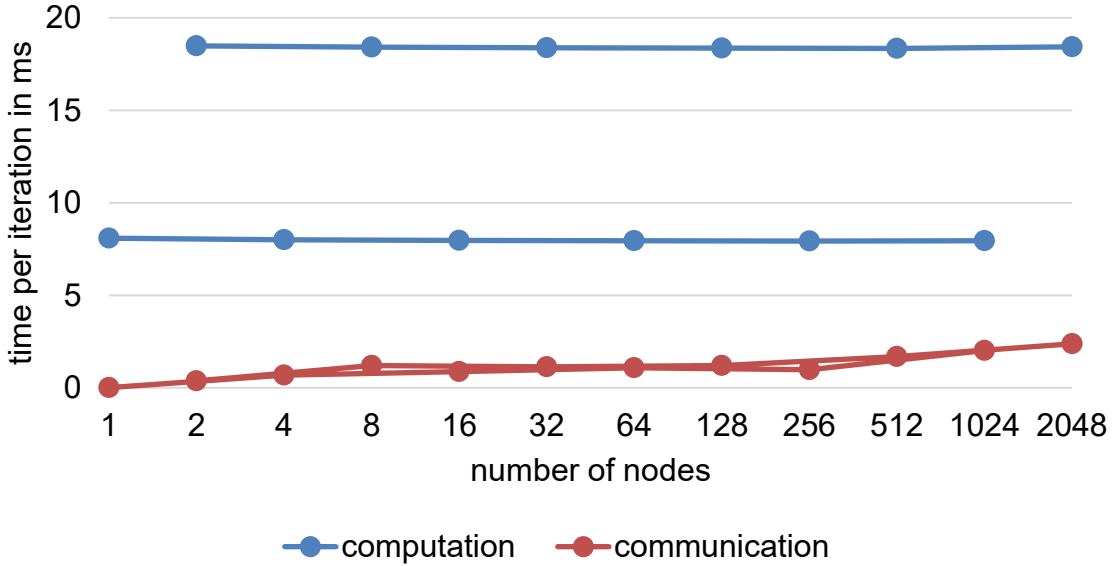


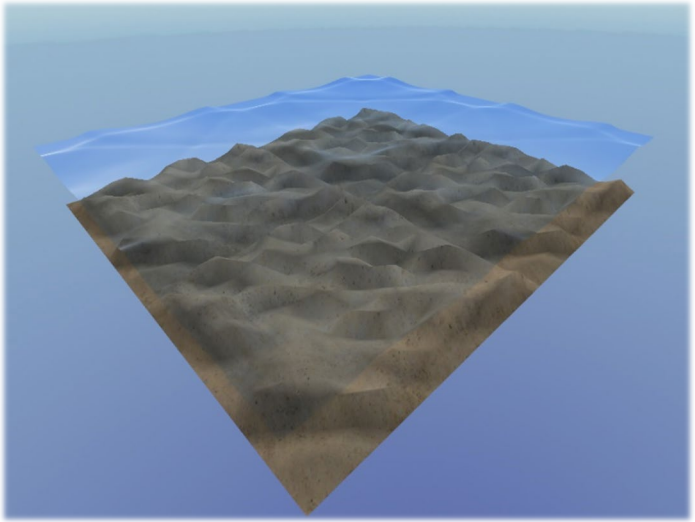
Figure: Definition of elevation and bathymetry

Aizinger, Dawson. *A discontinuous Galerkin method for two-dimensional flow and transport in shallow water*. Advances in Water Resources 25.1, 2002.

Evaluation on GPU cluster PizDaint

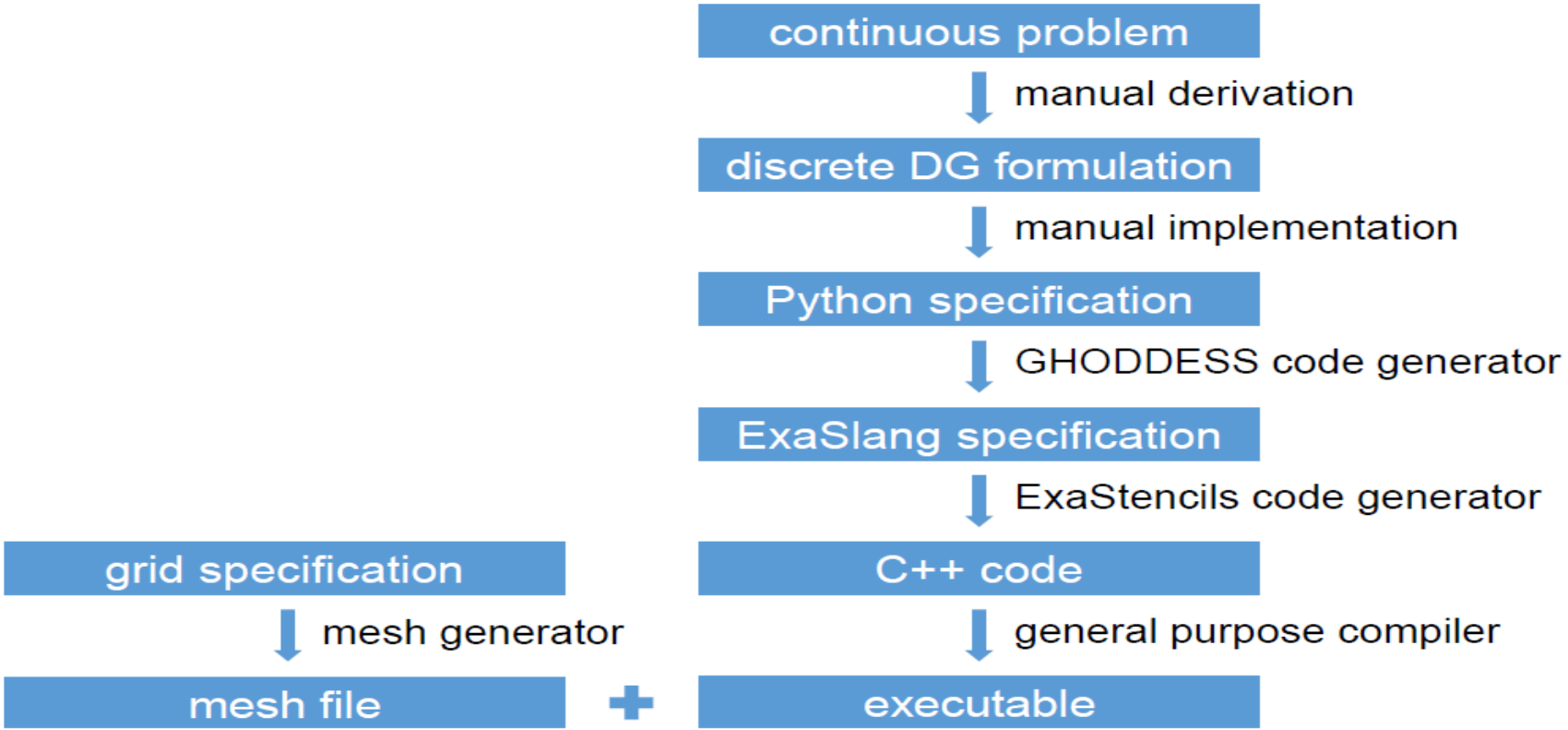
- Finite Volumes on a uniform grid is perfectly suited for ExaSlang



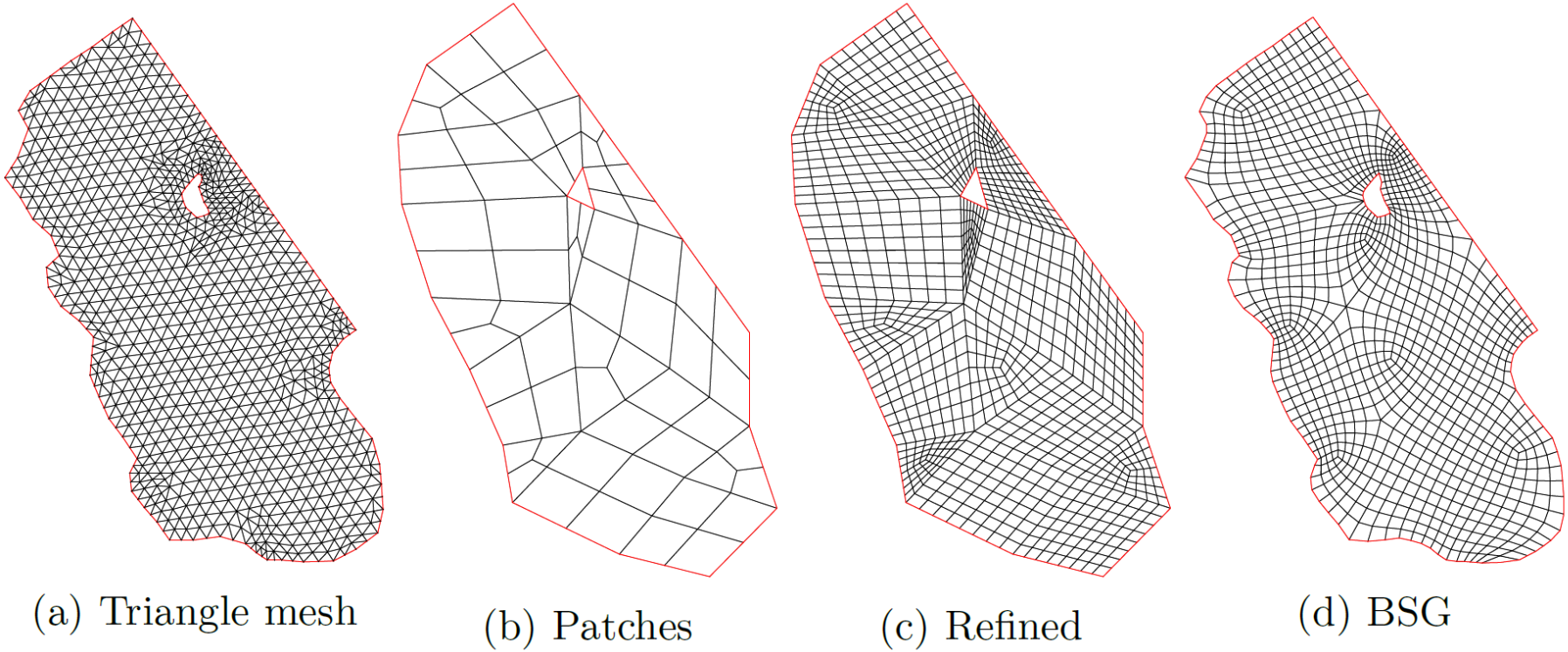


Kuckuk, Köstler. *Whole Program Generation of Massively Parallel Shallow Water Equation Solvers*. CLUSTER'18

Extended Toolchain (DFG project 2016-, 3 PhD students)



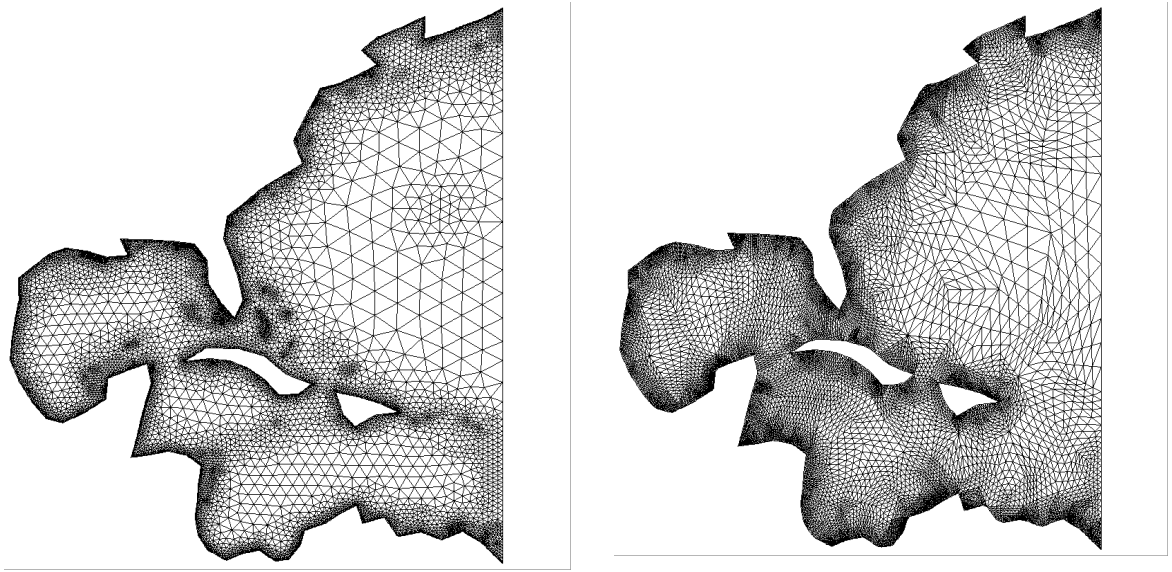
Block-structured grids in ExaStencils



Zint, Grosso. *Generation of Quadrilateral Block Structured Grids on Complex Domains for High Performance Simulation in Ocean Modeling,* 2020.

Numerical Results for Tide-driven Flow

Example: Flow at the US East coast with tidal forcing at open sea boundary



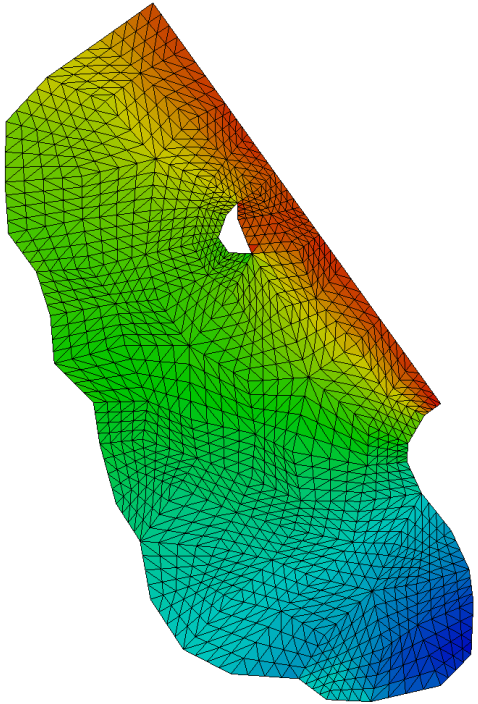
Finite element mesh with bathymetry for unstructured grid (left) and block-structured grid (right).

Reuter, Aizinger, Köstler. *A multi-platform scaling study for an OpenMP parallelization of a discontinuous Galerkin ocean model.* Computers & Fluids, 2015.

Required extensions

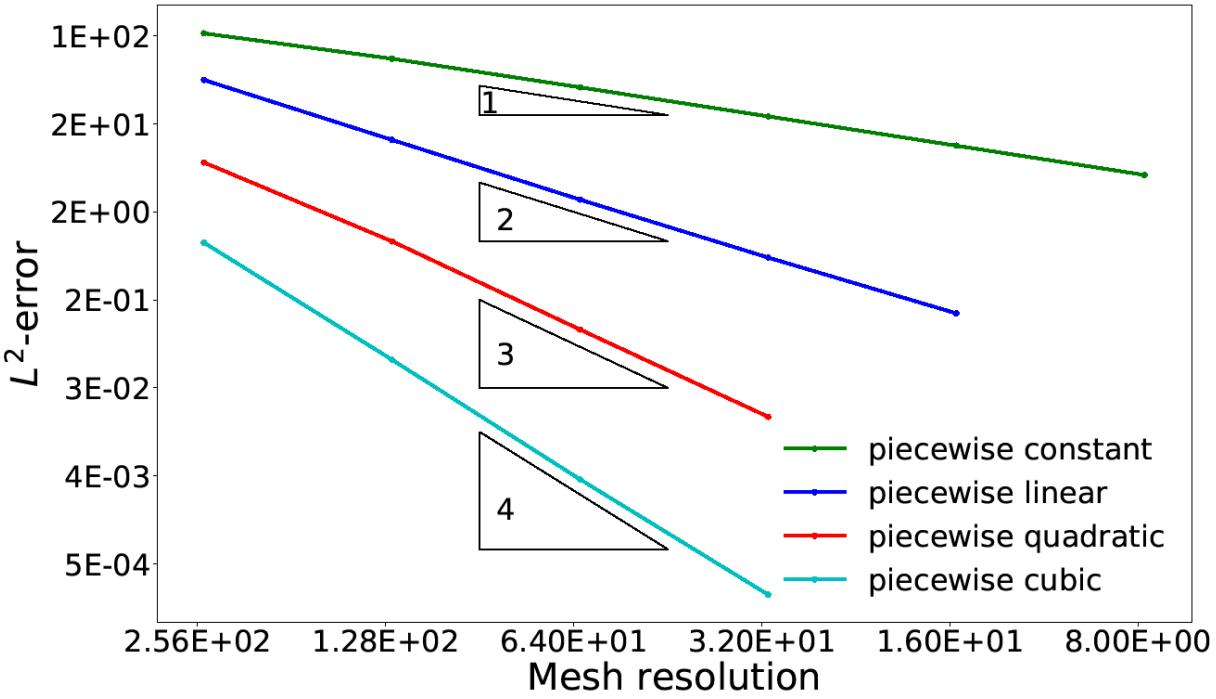
- Block-structured grids
  - Extension of the generator
- Higher order discretization: discontinuous Galerkin (DG)
  - Implementation as Python front end

$$
P_2 \begin{cases} P_1 \begin{cases} P_0 \begin{cases} \hat{\varphi}_1(\hat{\boldsymbol{x}}) = \sqrt{2} \\ \hat{\varphi}_2(\hat{\boldsymbol{x}}) = 2 - 6\hat{x}_1 \end{cases} \\ \hat{\varphi}_3(\hat{\boldsymbol{x}}) = 2\sqrt{3}(1 - \hat{x}_1 - 2\hat{x}_2) \end{cases} \\ \hat{\varphi}_4(\hat{\boldsymbol{x}}) = \sqrt{6}\big((10\hat{x}_1 - 8)\hat{x}_1 + 1\big) \\ \hat{\varphi}_5(\hat{\boldsymbol{x}}) = \sqrt{3}\big((5\hat{x}_1 - 4)\hat{x}_1 + (-15\hat{x}_2 + 12)\hat{x}_2 - 1\big) \\ \hat{\varphi}_6(\hat{\boldsymbol{x}}) = 3\sqrt{5}\big((3\hat{x}_1 + 8\hat{x}_2 - 4)\hat{x}_1 + (3\hat{x}_2 - 4)\hat{x}_2 + 1\big) \end{cases}
$$



Faghih-Naini, Kuckuk, Aizinger, Zint, Grosso, Köstler. *Towards whole program generation of quadrature-free discontinuous Galerkin methods for the shallow water equations.* Advances in Water Resources, 2020.

Convergence results for different orders

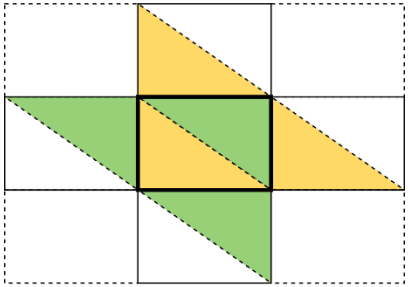


Mapping Math to Python

GHODDESS (Generation of Higher-Order Discretizations Deployed as ExaSlang Specifications)

- Uses Python library sympy[2] (analytical differentiation and integral evaluation)
- Contains classes representing triangles and data fields
- Supports quadrilateral grids only, where each element is divided into two differently oriented triangles in order to obtain a triangular grid
- Example: First part of element integral for ξ

$$\sum_{i=1}^{K(k)} \frac{c_{ei}^2}{|\det(\boldsymbol{B}_e)|} \left(B_{2,2}^e \int_{\hat{\Omega}} \frac{\partial \hat{\varphi}_p}{\partial \hat{x}_1} \hat{\varphi}_i \mathrm{d}\hat{x} - B_{2,1}^e \int_{\hat{\Omega}} \frac{\partial \hat{\varphi}_p}{\partial \hat{x}_2} \hat{\varphi}_i \mathrm{d}\hat{x} \right)$$

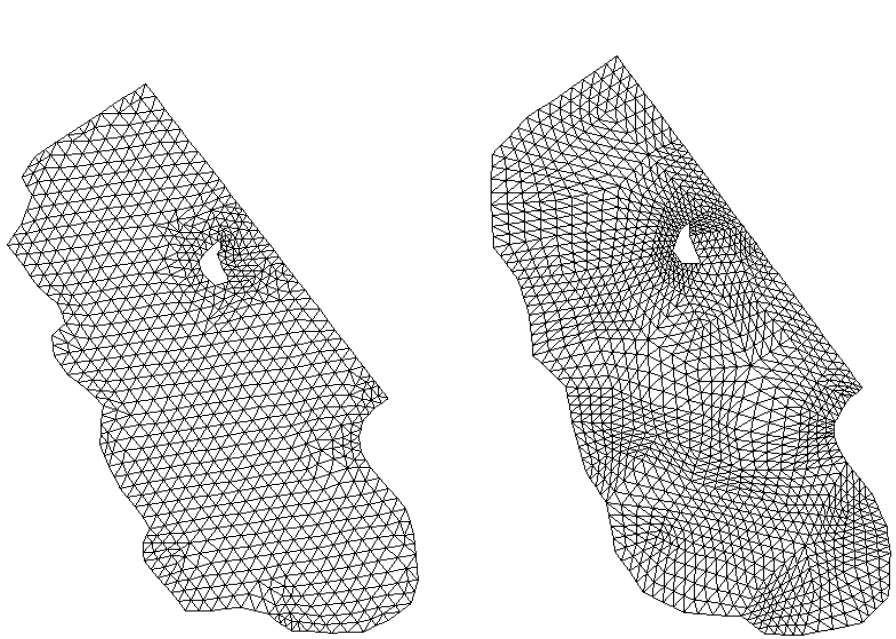


is translated to

```
sum( tri.b[1, 1] * cu(tri.orientation, k)
     * integrate_over_tri(basis.phi[k] * basis.phi_dx[p])
   - tri.b[1, 0] * cu(tri.orientation, k)
     * integrate_over_tri(basis.phi[k] * basis.phi_dy[p])
  for k in range(d)) * tri.det_b_inv
```

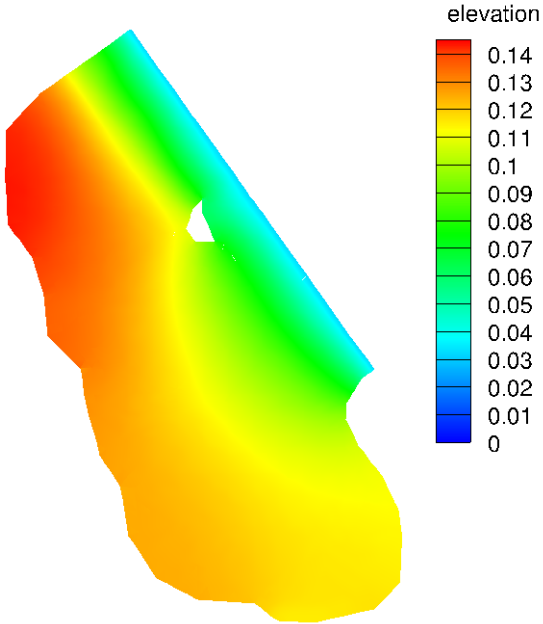
[2] https://www.sympy.org

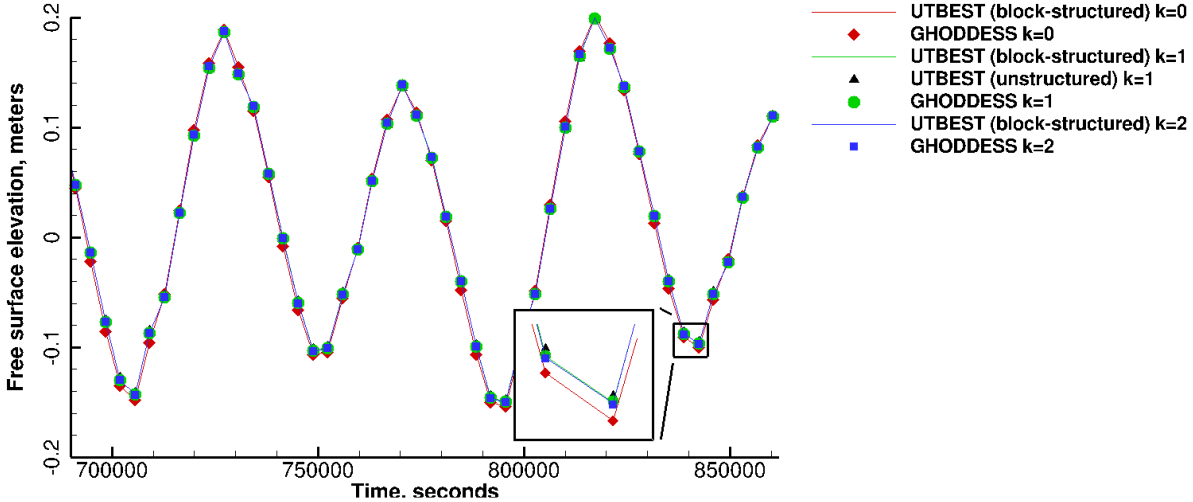
Tidal flow at Bahamas



Original UTBEST unstructured mesh (left), automatically generated block-structured mesh used by the GHODDESS framework (middle), bathymetry and positions of recording stations (right).

Numerical results for Bahamas



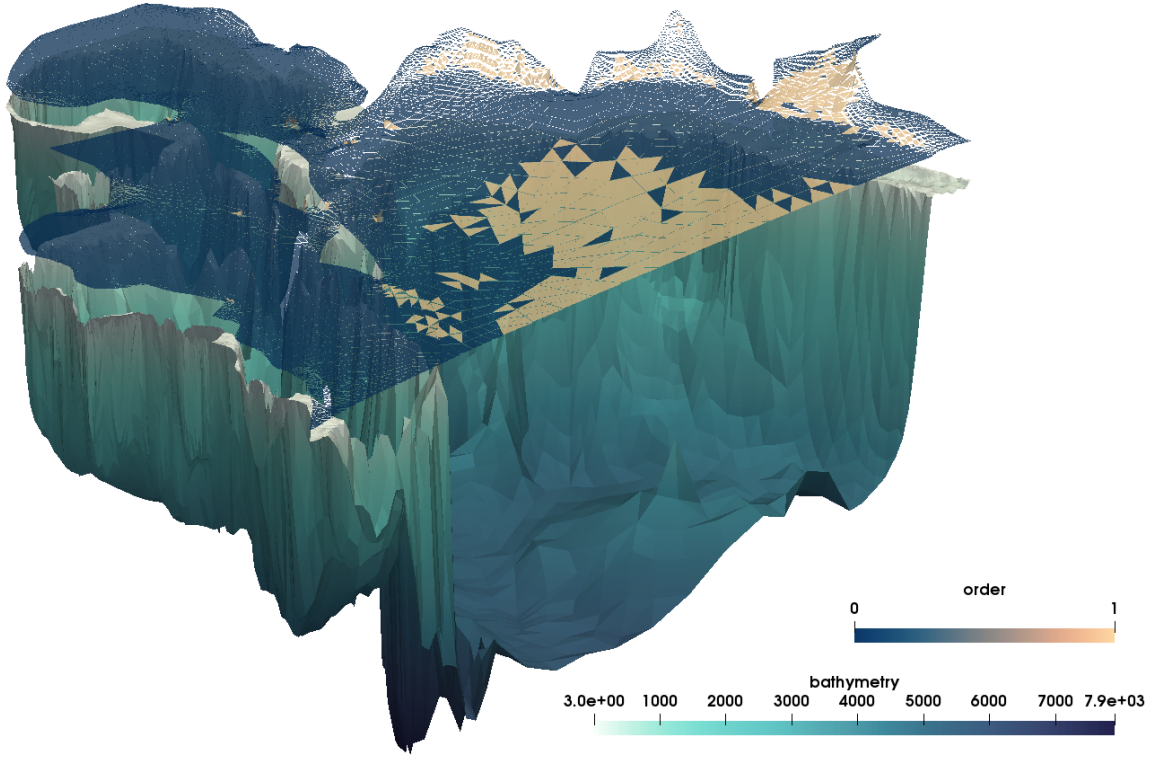


Runtimes per time step in ms for different scenarios

k	# elements	UTBEST (1)	GHODDESS (1)	GHODDESS (16)	α_{UT}
	Analytical example on square domain with perturbed mesh				
0	128	4.60E−02	1.94E−02	1.62E−01	2.38
	512	1.79E−01	6.63E−02	2.15E−01	2.69
	2 048	7.39E−01	2.42E−01	2.60E−01	3.05
	8 192	3.07E+00	9.87E−01	3.95E−01	7.77
	32 768	1.40E+01	3.93E+00	7.96E−01	17.6
1	128	3.15E−01	7.87E−02	3.19E−01	4.00
	515	1.23E+00	2.86E−01	4.11E−01	4.30
	2 048	4.96E+00	1.12E+00	6.21E−01	7.99
	8 192	2.00E+01	5.06E+00	1.14E+00	17.6
2	128	1.06E+00	5.84E−01	8.13E−01	1.31
	512	4.20E+00	2.09E+00	9.41E−01	3.85
	2 048	1.67E+01	8.93E+00	1.80E+00	8.15

k	# elements	UTBEST (1)	GHODDESS (1)	GHODDESS (16)	α_{UT}
	Tidal flow around Bahamas				
0	2634	4.24E−01	3.29E−01	7.33E−01	1.29
	10496	1.94E+00	8.65E−01	8.13E−01	2.39
	41984	1.07E+01	2.95E+00	1.20E+00	8.96
	167936	6.67E+01	1.30E+01	2.50E+00	26.61
1	2634	2.17E+00	2.10E+00	2.04E+00	1.06
	10496	1.05E+01	4.64E+00	2.35E+00	4.46
	41984	5.72E+01	1.99E+01	4.03E+00	14.2
	167936	3.21E+02	9.92E+01	1.62E+01	19.8
2	2634	1.15E+01	2.34E+01	6.08E+00	1.90
	10496	1.26E+02	4.21E+01	8.08E+00	15.6
	41984	7.29E+02	1.60E+02	2.18E+01	33.5
	167936	1.48E+03	8.11E+02	1.27E+02	11.6

p-adaptivity (US east coast)

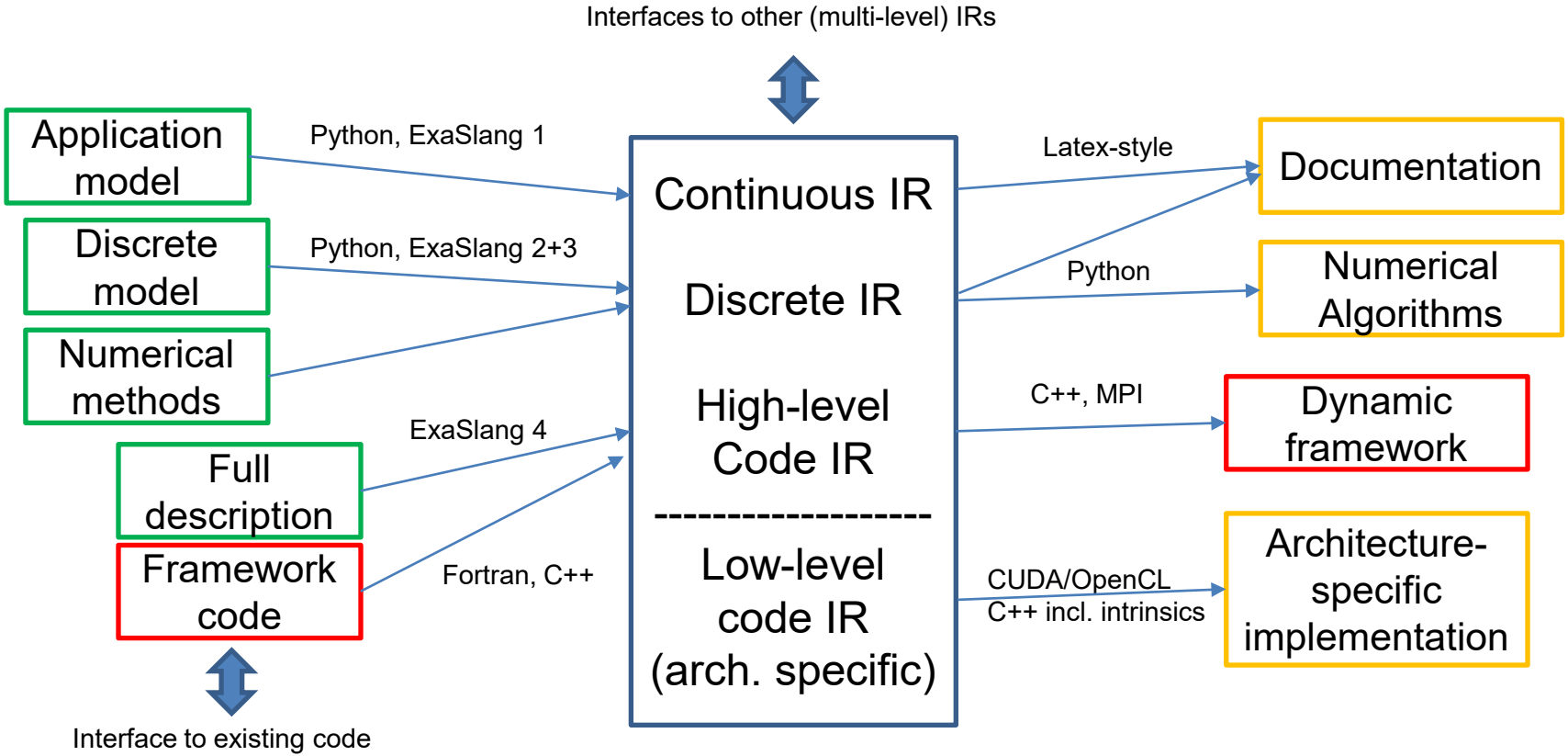


Conclusion

- The ExaSlang language stack and our code generation framework allows
  - Full program generation from domain-specific representations
  - **If** existing models and numerical methods are implemented or translated to ExaSlang
  - **If** the underlying block-structured grids can be used
  - And is also fast, **if** the required domain-specifc optimizations are integrated in the code generator
  - Next: provide interfaces to other technologies and codes!

Towards dynamic HPC software frameworks

Proposed Toolchain (DFG project 2020-, 6 PhD students + 1 PostDoc)



MITgcm/seaice Coupling

momentum equation

$$m\frac{D\boldsymbol{u}}{Dt} = -mf\boldsymbol{k}\times\boldsymbol{u} + \tau_{air} + \tau_{ocean} - m\nabla\Phi(0) + \nabla\cdot\sigma$$

shear stress terms

$$\tau_{ocean/air} = \rho_{ocean/air} C_{ocean/air} |\mathbf{U}_{ocean/air} - \mathbf{u}| R(\mathbf{U}_{ocean/air} - \mathbf{u})$$

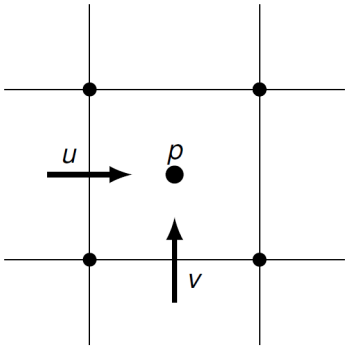


Figure: The staggered C-grid used by MITgcm and seaice

http://mitgcm.org/

Fortran framework integration

- Analog to OpenMP (C$OMP) and OpenACC (C$ACC) annotations
- ExaSlang 4 code with extra modifiers if necessary
- Steps:
  - parse Fortran code in all caps but keep case for annotations
  - sort and merge individual variable/constant/field declaration statements
  - progress to layer 4 IR
  - drop arguments and globals
  - convert absolute array index with relative offset
  - insert constants, simplify expression, remove loop variable
  - if annotated replace with given layer 4 code using parser
  - case insensitive name resolution of globals fields, global variables and function calls
  - Fortran backend for ExaStencils code generation framework

Example

Abstract formulation

```
res = Laplace * U
return max(res)
```

Fortan code

```
!$EXA Function Residual@all() : Double
      Real*8 function Residual()
       implicit none

       Integer NPoints, i, j
       Real*8 norm, U, RHS, RES, C, N, S, W, E
       Parameter(NPoints=42)
       Dimension U(0:NPoints+1, 0:NPoints+1)
       Dimension RHS(NPoints, NPoints)
       Dimension RES(NPoints, NPoints)
       Dimension C(NPoints, NPoints)
       Dimension N(NPoints, NPoints)
       Dimension S(NPoints, NPoints)
       Dimension W(NPoints, NPoints)
       Dimension E(NPoints, NPoints)
       Common /fields/ U, RHS, RES, C, N, S, W, E

       norm = 0
!$EXA loop over RES with reduction(max: norm) collapse(2)
       DO i = 1, NPoints
        DO j = 1, NPoints
         res(i,j) = rhs(i,j)-( C(i,j)*U(i,j) +
     &              N(i,j)*U(i-1,j) + S(i,j)*U(i+1,j) +
     &              W(i,j)*U(i,j-1) + E(i,j)*U(i,j+1) )
         norm = max(abs(res(i,j)), norm)
        ENDDO
       ENDDO

       Residual = norm
      end function
```

generated layer 4 code

```
Function Residual@all : Double {
        Var RESIDUAL : Double
        Var I : Integer
        Var J : Integer
        Var NORM : Double
        Val NPOINTS : Integer = 42

        NORM = 0
        loop over RES with reduction ( max : NORM ) {
          RES@[0, 0] = ( RHS@[0, 0] - ( ( ( ( ( C@[0, 0] * U@[0, 0] ) +
                       (N@[0, 0] * U@[-1, 0] ) ) + ( S@[0, 0] * U@[1, 0] ) ) +
                       ( W@[0, 0] * U@[0, -1] ) ) + ( E@[0, 0] * U@[0, 1] ) ) )
           NORM = max ( abs ( RES@[0, 0] ), NORM )
        }
        RESIDUAL = NORM
        return RESIDUAL
}
```

Future Work

- Performance Portability: Sustained performance engineering
- Higher-order DG: Optimize p-adaptivity
- Parallel Data structures: Extend possible grid types
- New Applications: e.g. Tsunami, storm surge (add wetting/drying), particles
- AI Integration: Auto-tuned numerical methods
- Dynamic framework: Code Generation for Automatic Interfaces, MLIR
- Collaborative work with Peano, DUNE and MITgcm
- Connect to other code generation approaches in climate simulation
- Better accessibility – documentation & tutorials

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  - Bundesministerium für Bildung und Forschung
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  - DFG SPP 1648/1 – Software for Exascale computing

KONWIHR II

Bundesministerium für Bildung und Forschung

des Bundesministeriums für Bildung und Forschung von Richtlinien zur Förderung von Forschungsvorhaben auf dem Gebiet "HPC-Software für skalierbare Parallelrechner" im Rahmen des Förderprogramms "IKT 2020 - Forschung für Innovationen"

NVIDIA CUDA RESEARCH CENTER

DFG Deutsche Forschungsgemeinschaft

ExaStencils

https://www.exastencils.fau.de/

SPPEXA

  - DFG Projekt Projekts *Vollständig-generierte adaptive Methoden höherer Ordnung für Ozeanmodellierung auf block-strukturierten Gittern and Dynamische HPC Softwarepakete: Nahtlose Integration von existierenden Softwarepaketen und Codegenerierungstechniken*
  - *Supercomputing centers*

Tokyo Institute of Technology ATTUNE

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JÜLICH FORSCHUNGSZENTRUM

CSCS Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre

Thank you for your attention!

ExaStencils is now open source:

https://i10git.cs.fau.de/exastencils/release