Metaprogramming for CSE Applications meets performance engineering

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Contents

- Motivation
- ExaStencils Code Generation Framework
  - Applications
  - Performance Engineering
- Next: Metaprogramming

Code generation and Metaprogramming

Definition: Code generation in a strict sense is used to describe the process of producing code that can be executed on a certain platform from an abstract representation

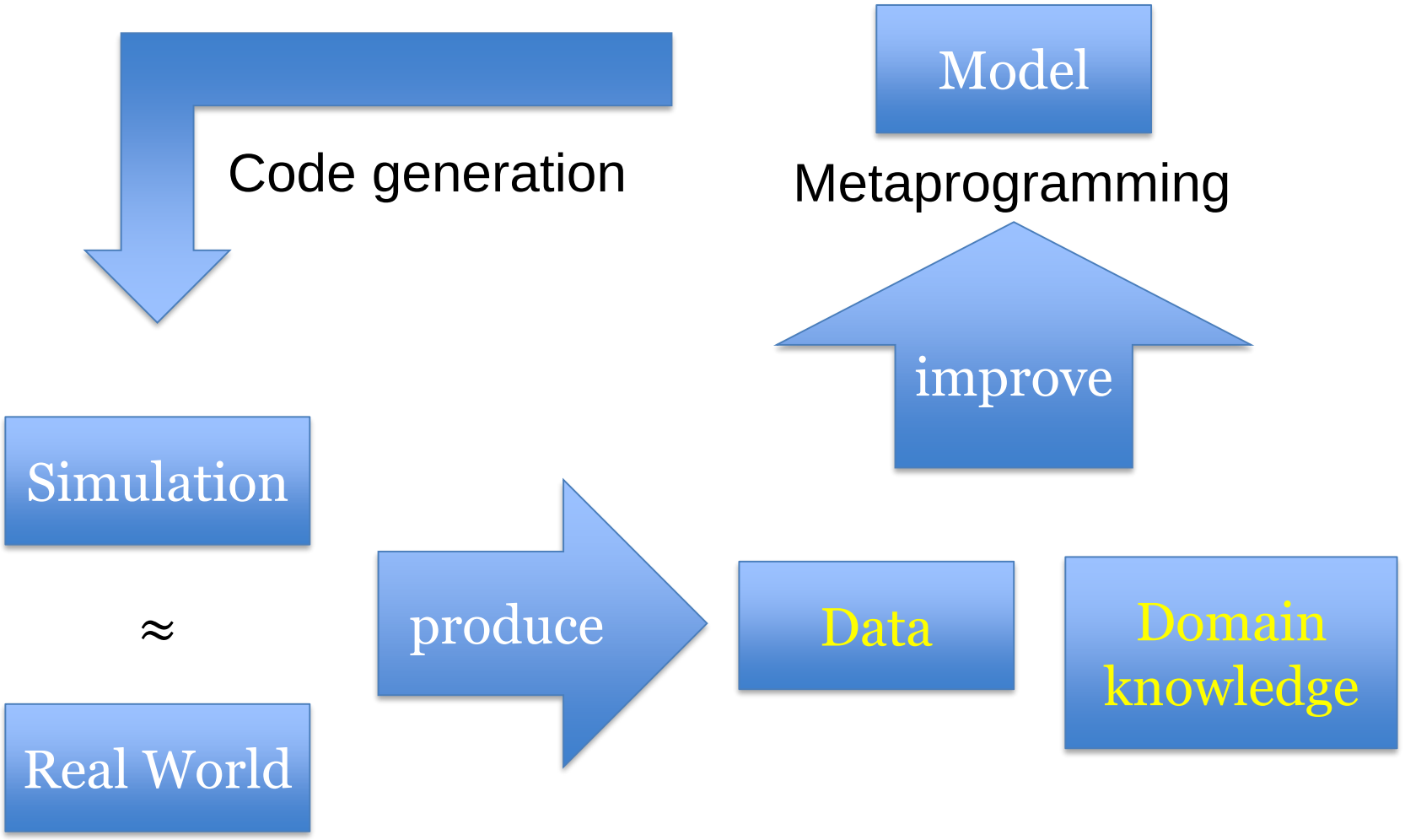
Why? Because programming is time-consuming.

Definition: Metaprogramming is a very general term and can be defined as writing software that can itself produce new software.

The final goal is to develop software that can itself solve problems without human interaction.

Approaches: Genetic Programming, Deep Learning

CSE optimization problem



Metaprogramming group @ LSS

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- Code generation
  - Parallel Data Structures
  - Performance engineering
  - GPU, accelerators
- Metaprogramming
  - Lisp, AnyDSL
  - Scala
  - Python, llvm
  - C++
  - Genetic Programming, Deep Learning
- Applications
  - Data analysis, medical image processing
  - Solvers for PDEs, DG discretizations
  - Tsunami simulation, material sciences, CFD

ExaStencils

SPPEXA

SKAMPY

METACCA

HPC²SE

DAAD

DFG Deutsche Forschungsgemeinschaft

The ExaStencils Framework

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Project ExaStencils

- Sebastian Kuckuk
- Georg Altmann
- Harald Köstler
- Ulrich Rüde

- Alexander Grebhahn
- Sven Apel

- Christian Schmitt
- Frank Hannig
- Jürgen Teich

- Hannah Rittich
- Lisa Claus
- Matthias Bolten

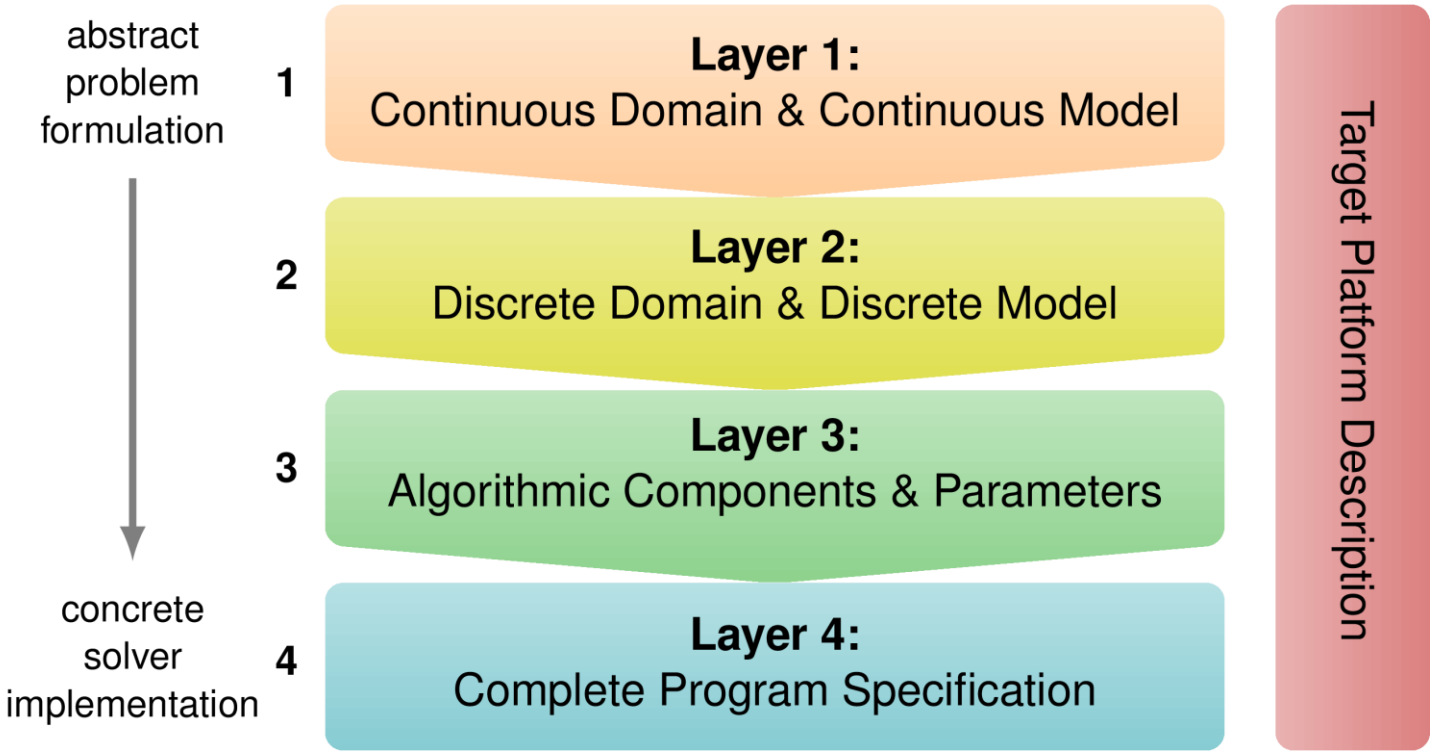
- Stefan Kronawitter
- Armin Größlinger
- Christian Lengauer

What is ExaStencils?

- Scope:
  - (Geometric) **multigrid solvers** for
  - Finite difference and finite volume discretizations of **elliptic PDEs**
  - On regular (staggered) quad and hex meshes
- **Multi-layered, external DSL** as input, whole program as output
- Transformation-based **code generation framework** written in Scala
- Support for OpenMP, MPI and/or CUDA
- Many **optimizations can be applied automatically** (loop transformations, vectorization, sophisticated CSE, etc.)
- Applications from **CFD**, image processing and quantum chemistry

ExaSlang

- We propose a multilayered, external DSL



Schmitt, Kuckuk, Hannig, Köstler, Teich. **ExaSlang: A Domain-Specific Language for Highly Scalable Multigrid Solvers**.

Workflow

Setup
- User writes DSL code and sets up configuration files

Gener.
- Code generator emits source code in target language and, optionally, a Makefile, project file, job script, etc.

Comp.
- User moves generated code to target machine and uses general purpose compilers

Run
- User executes the code and checks results

```
/** Layer 2 **/

// domain - information is carried over from L1
Domain global

// fields from L1
Field Solution@all with Real on Node of global = 0.0
Field RHS@all with Real on Node of global = 0.0

// boundary conditions from L1
Field Solution@finest on boundary = vf_boundaryCoord_x**2 - 0.5 * …
Field Solution@(all but finest) on boundary = 0.0

// (discretized) operators from L1
Operator Laplace from Stencil {
  [ 0,  0] =>  2.0 / ( vf_gridWidth_x ** 2 ) + 2.0 / ( vf_gridWidth_y ** 2 )
  [-1,  0] => -1.0 / ( vf_gridWidth_x ** 2 )
  [ 1,  0] => -1.0 / ( vf_gridWidth_x ** 2 )
  [ 0, -1] => -1.0 / ( vf_gridWidth_y ** 2 )
  [ 0,  1] => -1.0 / ( vf_gridWidth_y ** 2 )
}
```

```
/** Layer 3 **/

/* fields and operators from L2 are progressed automatically */

// new fields
Field Residual      from Solution

// override inherited boundary conditions where applicable
override bc for Residual@finest with 0.0

// generate default inter-grid operators for node-based discretizations
Operator RestrictionStencil from default restriction on Node with 'linear'
Operator CorrectionStencil from default prolongation on Node with 'linear'

// create smoother function
Function Smoother@all {
  Val omega : Real = 0.8
  repeat 3 times {
    Solution =
      Solution + omega * diag_inv ( Laplace ) * ( RHS - Laplace * Solution )
  }
}
```

```
/** Layer 3 **/

// create v-cycle function
Function VCycle@((coarsest + 1) to finest) {
  Smoother ( )

  Residual = RHS - ( Laplace * Solution )
  RHS@coarser = RestrictionStencil * Residual

  Solution@coarser = 0.0
  VCycle@coarser ( )

  Solution += CorrectionStencil * Solution@coarser

  Smoother ( )
}

Function VCycle@coarsest {
  /* CGS */
}
```

```
/** Layer 4 **/

// create main function
Function Application ( ) : Unit {
    /* init code */

    Var resStart : Real = NormResidual@finest ( )
    Var curRes   : Real = resStart

    repeat until res_0 < 1.0E-5 * resStart_0 {
        VCycle@finest ( )
        curRes = NormResidual@finest ( )
    }

    /* de-init code */
}
```

Vanka-Type smoothers on L4

```
loop over p {
  solve locally {
    u@[0, 0, 0] => A_u@[0, 0, 0] * u@[0, 0, 0] == rhs_u@[0, 0, 0]
      + vf_cellWidth_y * vf_cellWidth_z * ( p@[-1, 0, 0] - p@[0, 0, 0] )
    u@[1, 0, 0] => A_u@[1, 0, 0] * u@[1, 0, 0] == rhs_u@[1, 0, 0]
      + vf_cellWidth_y * vf_cellWidth_z * ( p@[ 0, 0, 0] - p@[1, 0, 0] )

    v@[0, 0, 0] => A_v@[0, 0, 0] * v@[0, 0, 0] == rhs_v@[0, 0, 0]
      + vf_cellWidth_x * vf_cellWidth_z * ( p@[0, -1, 0] - p@[0, 0, 0] )
    v@[0, 1, 0] => …

    w@[0, 0, 0] => A_w@[0, 0, 0] * w@[0, 0, 0] == rhs_w@[0, 0, 0]
      + vf_cellWidth_x * vf_cellWidth_y * ( p@[0, 0, -1] - p@[0, 0, 0] )
    w@[0, 0, 1] => …

    p@[0, 0, 0] => rhs_p ==
        integrateOverEastFace  ( u * rho ) - integrateOverWestFace   ( u * rho )
      + integrateOverNorthFace ( v * rho ) - integrateOverSouthFace  ( v * rho )
      + integrateOverTopFace   ( w * rho ) - integrateOverBottomFace ( w * rho )
  }
}
```

Applications: It is all about Grids

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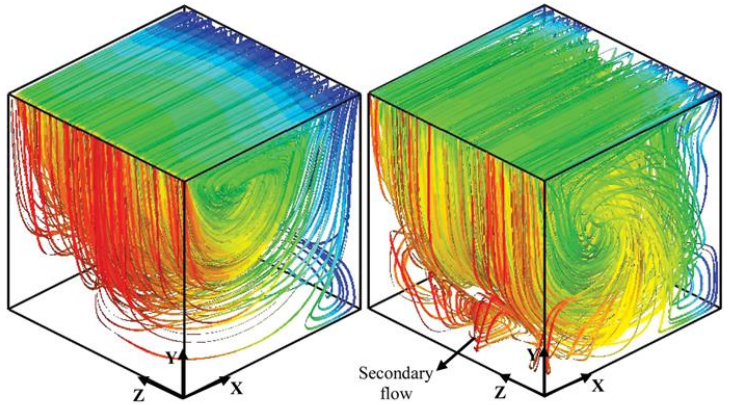
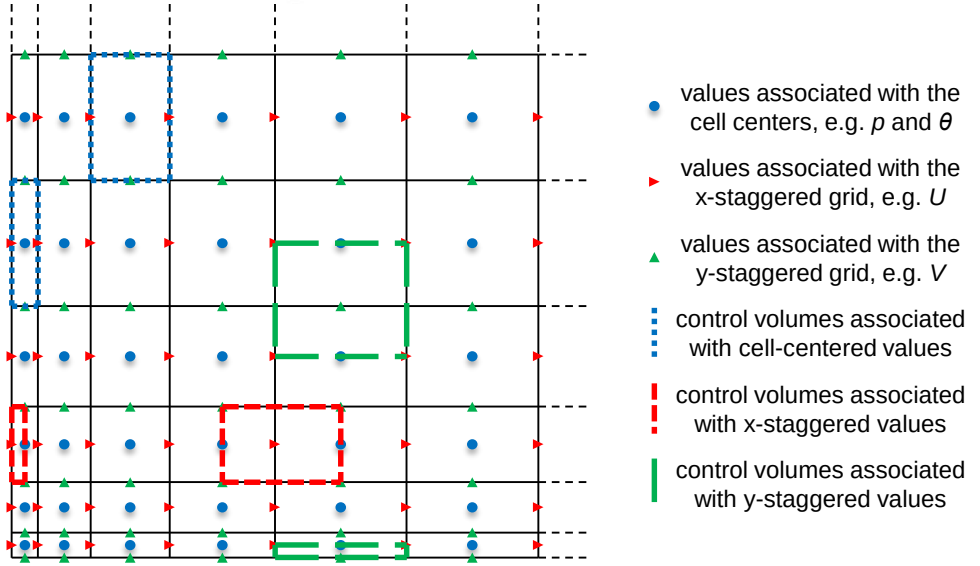
Showcase

- Work with Haase (U. Graz) and Vasco (U. Santiago de Chile)
- Simulation of non-Newtonian/non-isothermal fluids
- 3D FV discretization of staggered grids
- Recent extension towards FAS-FMG
- (Automatic) parallelization using OMP/MPI/CUDA





Vasco, Moraga, Haase. **Parallel finite volume method simulation of three-dimensional fluid flow and convective heat transfer for viscoplastic non-Newtonian fluids**
Kuckuk, Haase, Vasco, Köstler. **Towards Generating Efficient Flow Solvers with the ExaStencils Approach**

Scope: Towards Ocean Simulation

- Overall goal: simulation of ocean behavior
- Discretization using discontinuous Galerkin (DG) methods
- Performance and scalability

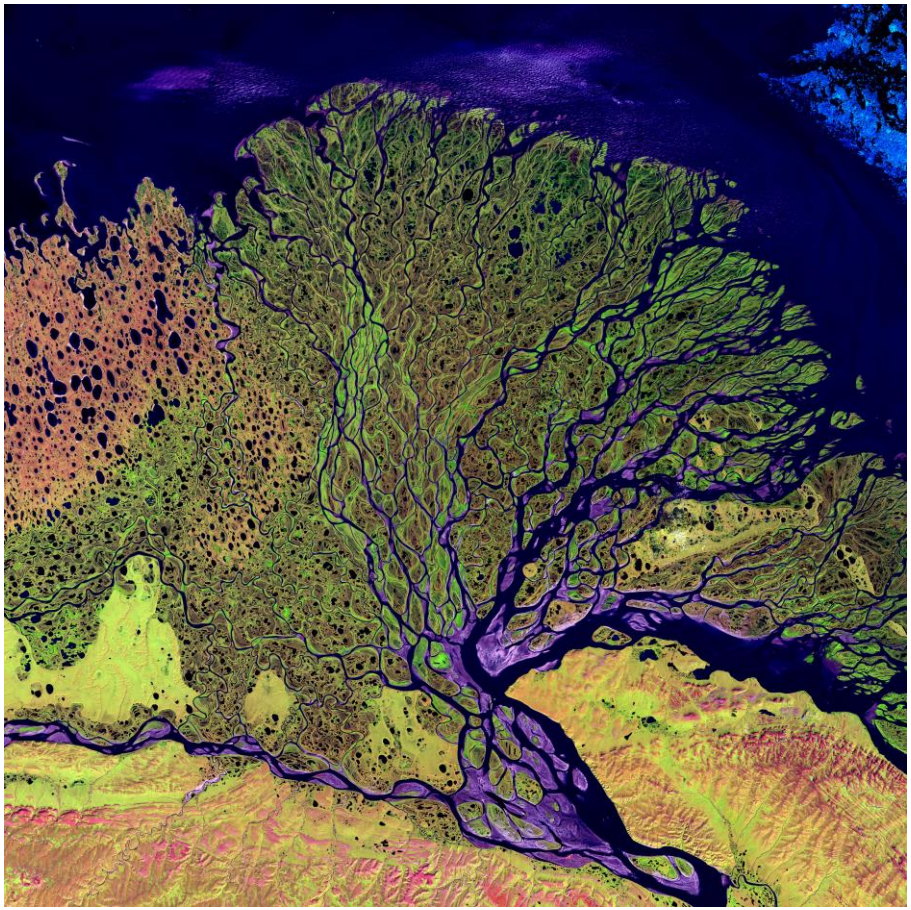


Image credits: NASA Landsat

Hybrid Grids: Unstructured Grids are slow(er)!

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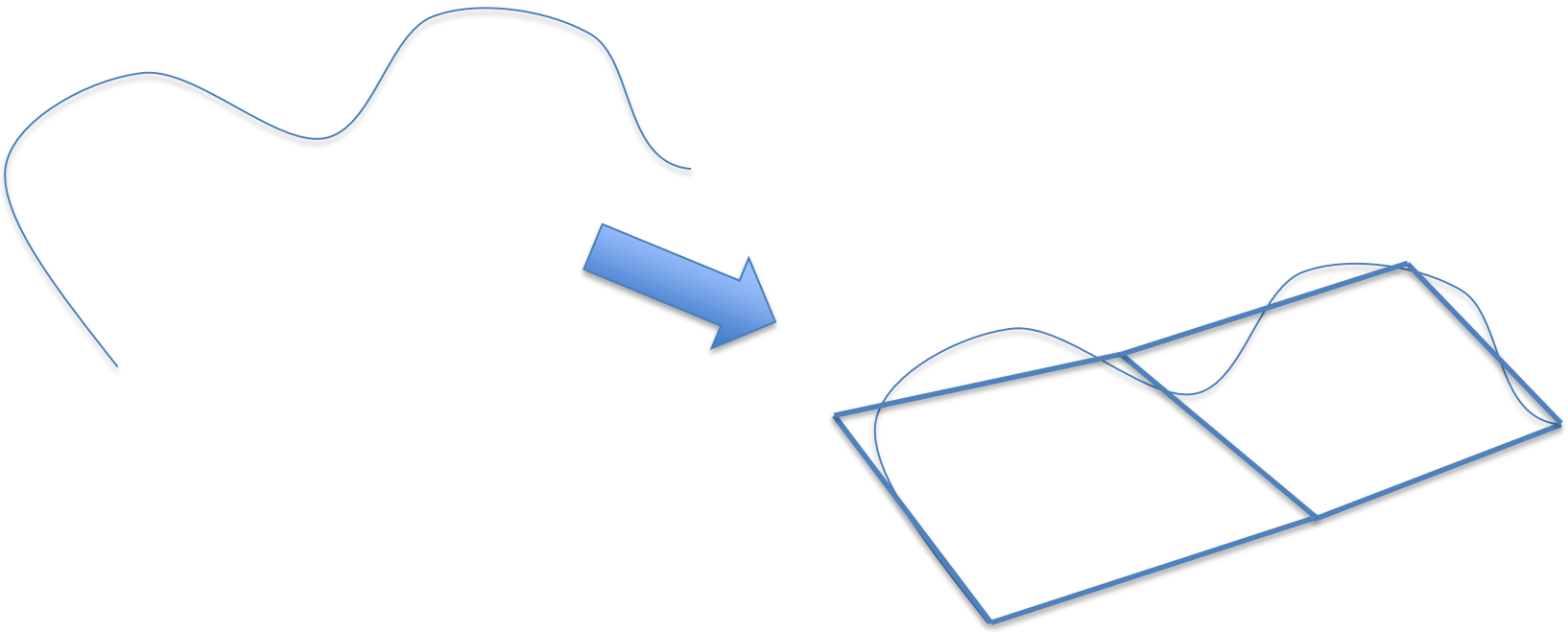
Generation of Block-Structured Grids

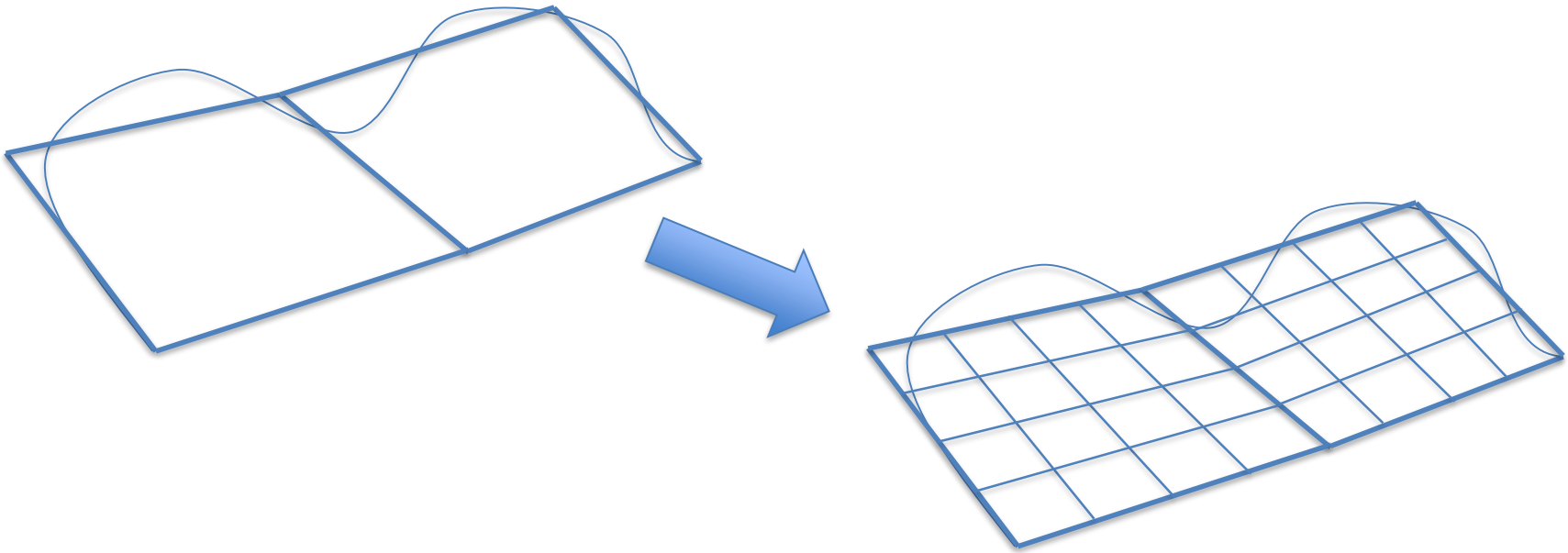
1. Rough (unstructured) tessellation of the computational domain



For illustration purposes only!

Generation of Block-Structured Grids

1. Rough (unstructured) tessellation of the computational domain
2. Uniform subdivision



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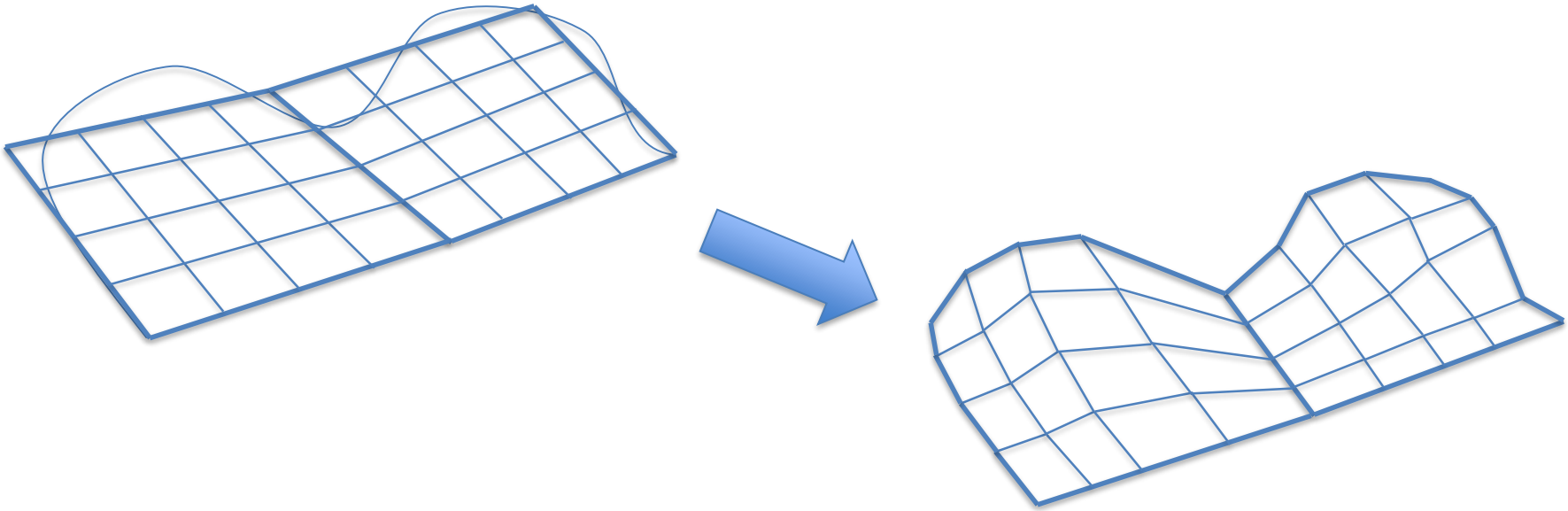
Generation of Block-Structured Grids

1. Rough (unstructured) tessellation of the computational domain
2. Uniform subdivision
3. Adaptation of vertex positions



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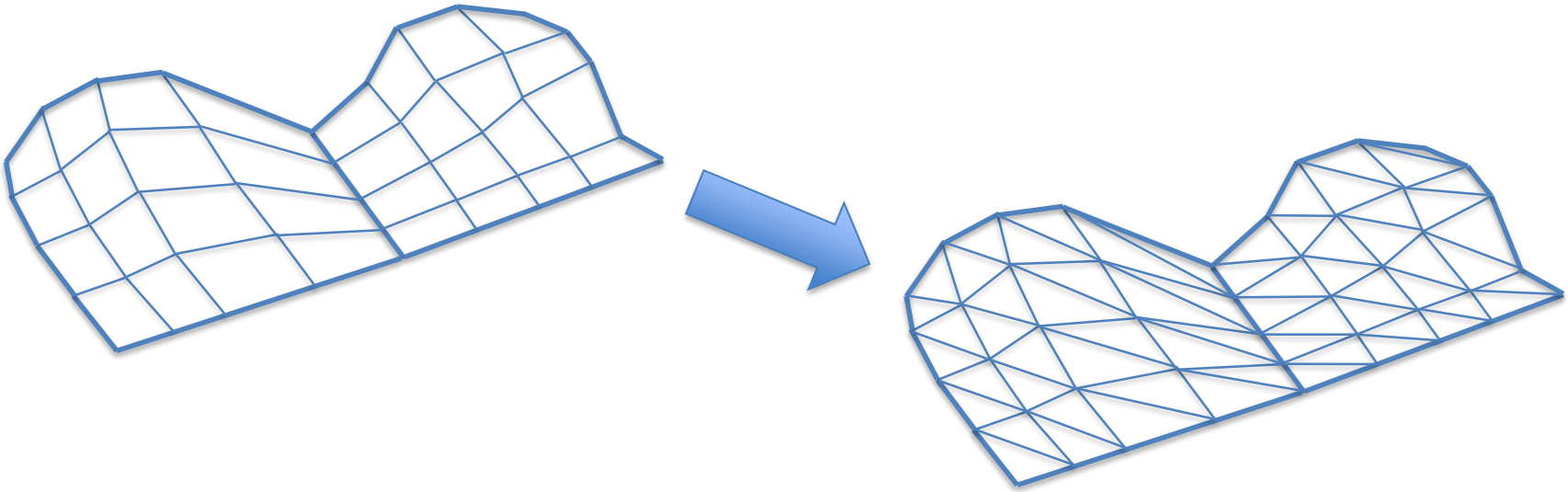
Generation of Block-Structured Grids

1. Rough (unstructured) tessellation of the computational domain
2. Uniform subdivision
3. Adaptation of vertex positions
4. Triangulation



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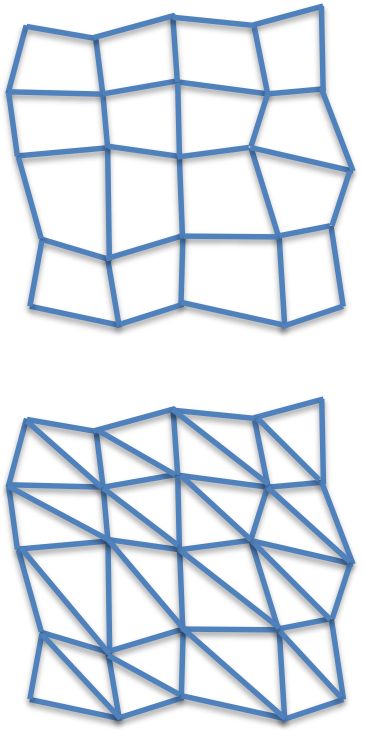
Current State

- What is already possible?
  - Finite volume discretizations for simple model problems on regular, non-uniform patches (cell-centered, 2D)
  - Using the complete ExaStencils pipeline
- What is missing?
  - Suitable abstractions and language extensions for DG
  - Extension to prisms
  - (Specialized) communication routines for triangle and prism data



Towards Performance Engineering

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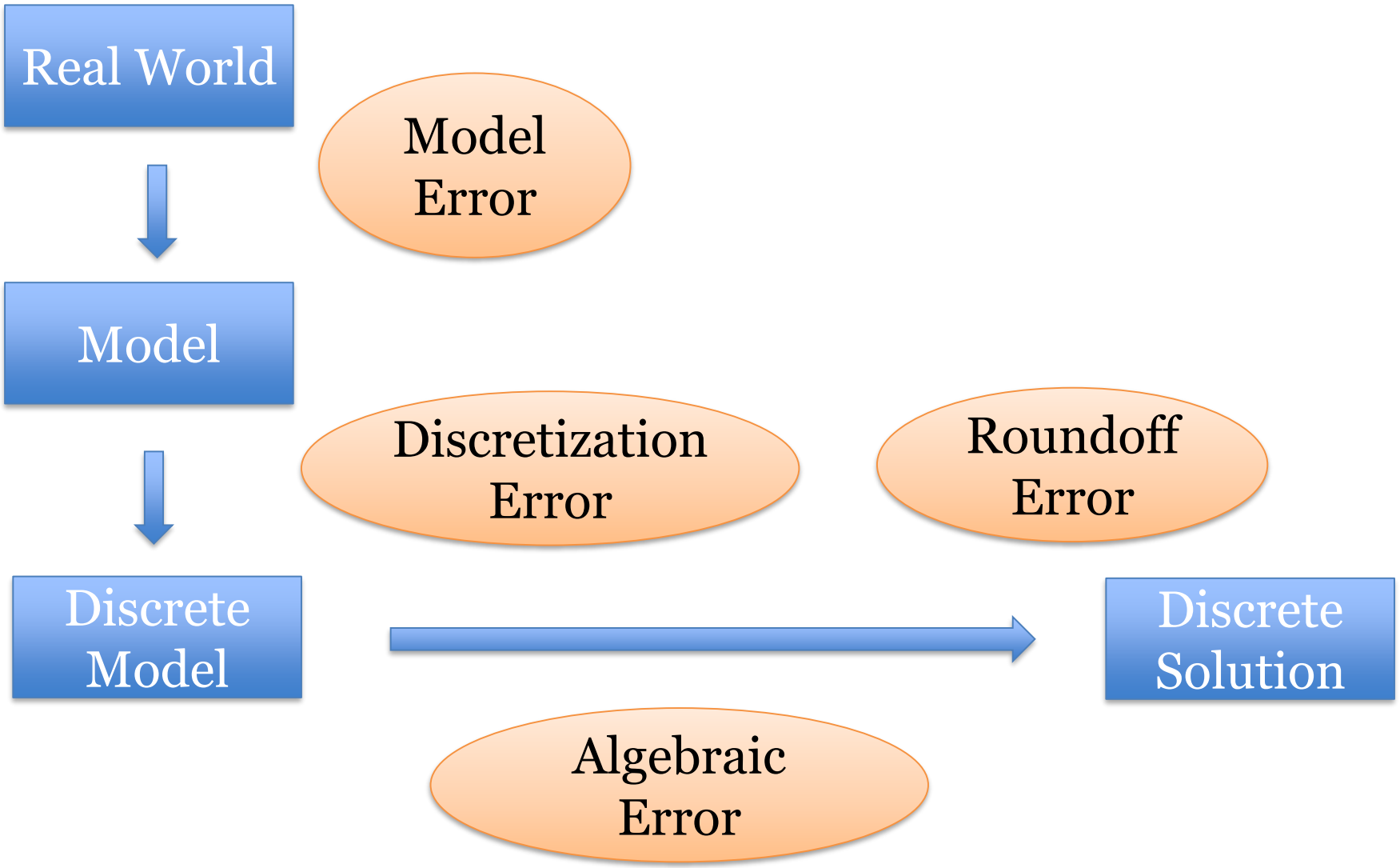
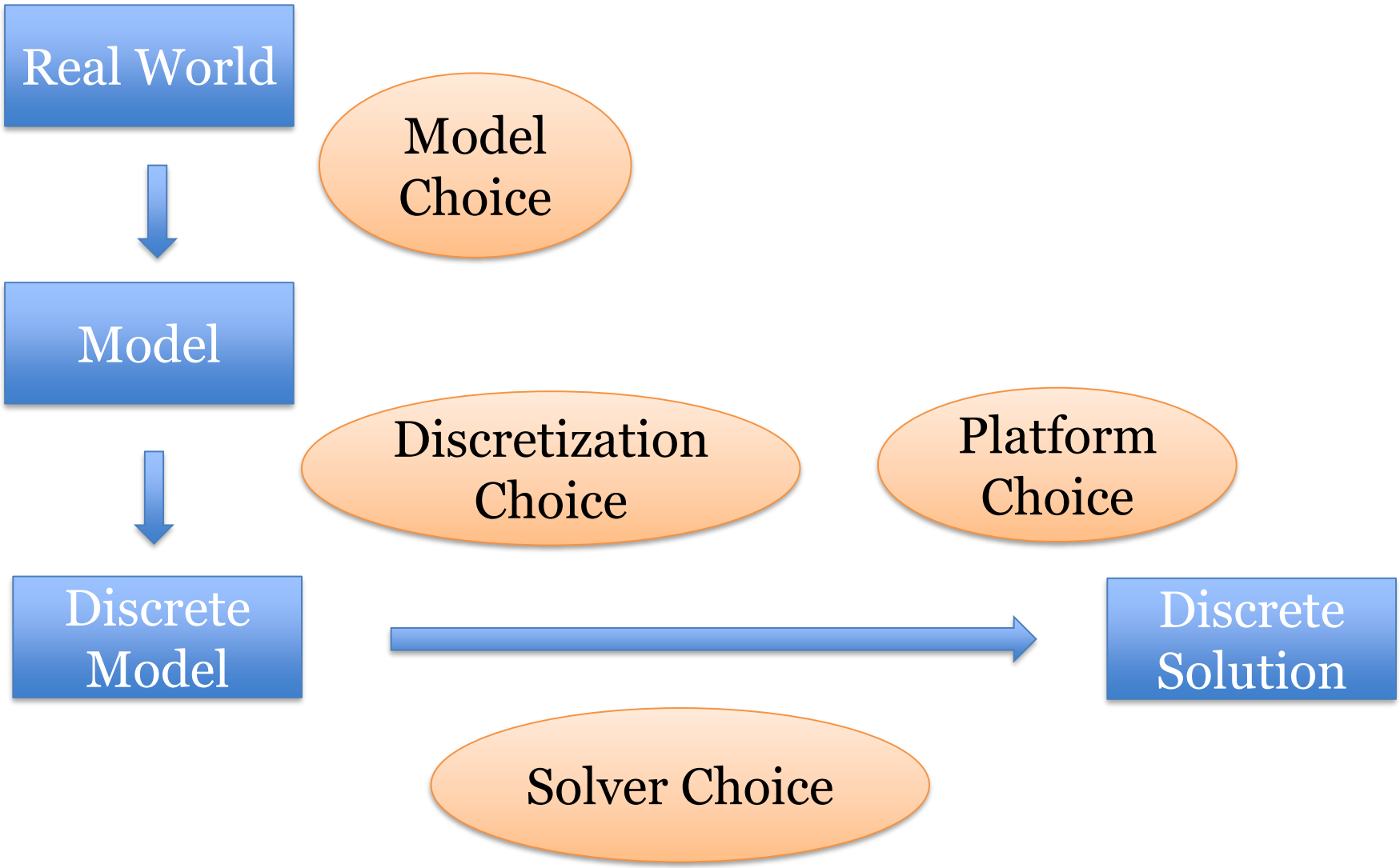
Error Types


Real World
Model Error
Model
Discretization Error
Roundoff Error
Discrete Model
Discrete Solution
Algebraic Error

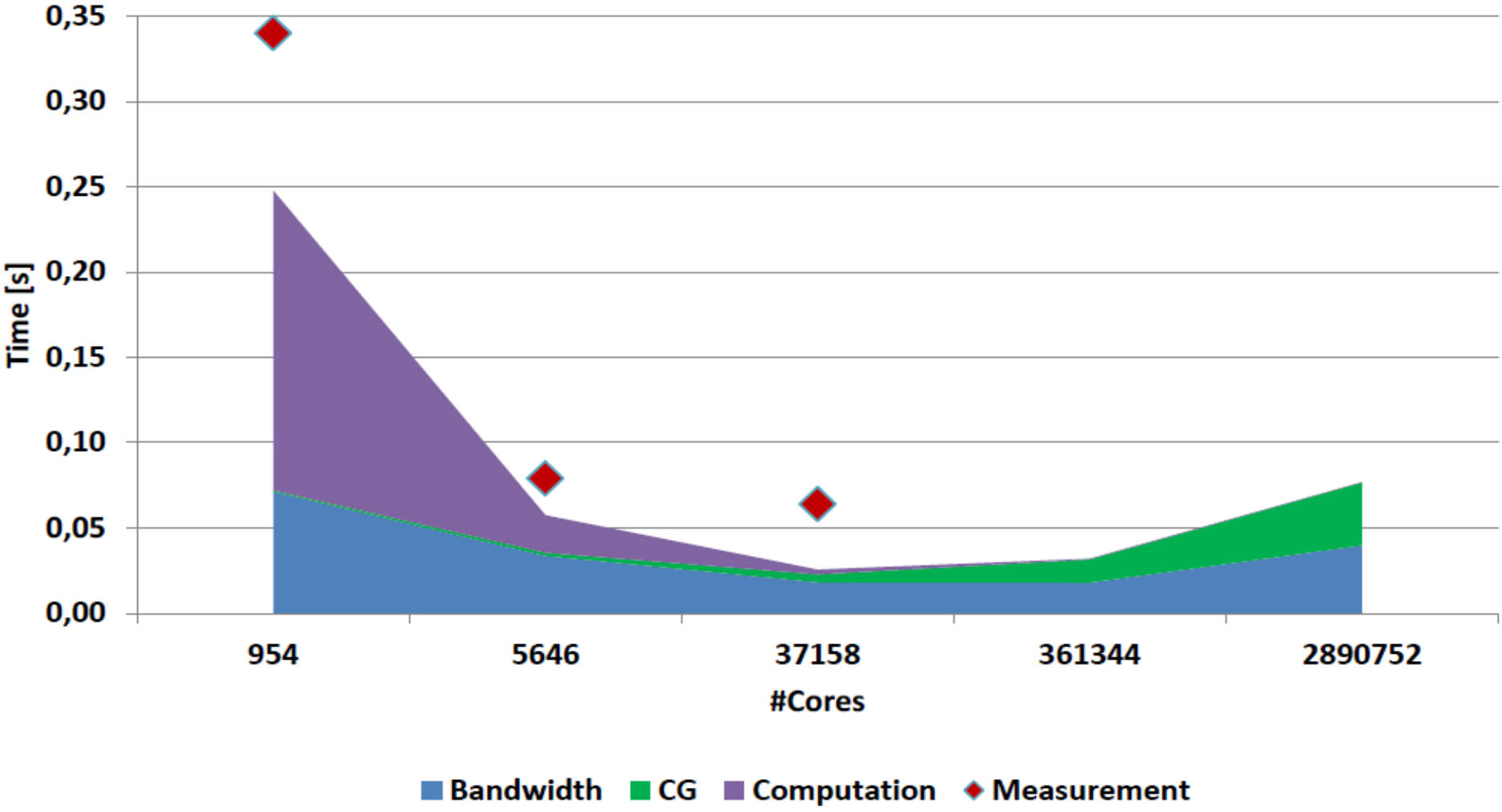
Algorithmic Performance Engineering



Optimization Problem

- For each choice you require a valid performance model that estimates the runtime for your settings!
- Therefore there is a need to automize the creation of performance models

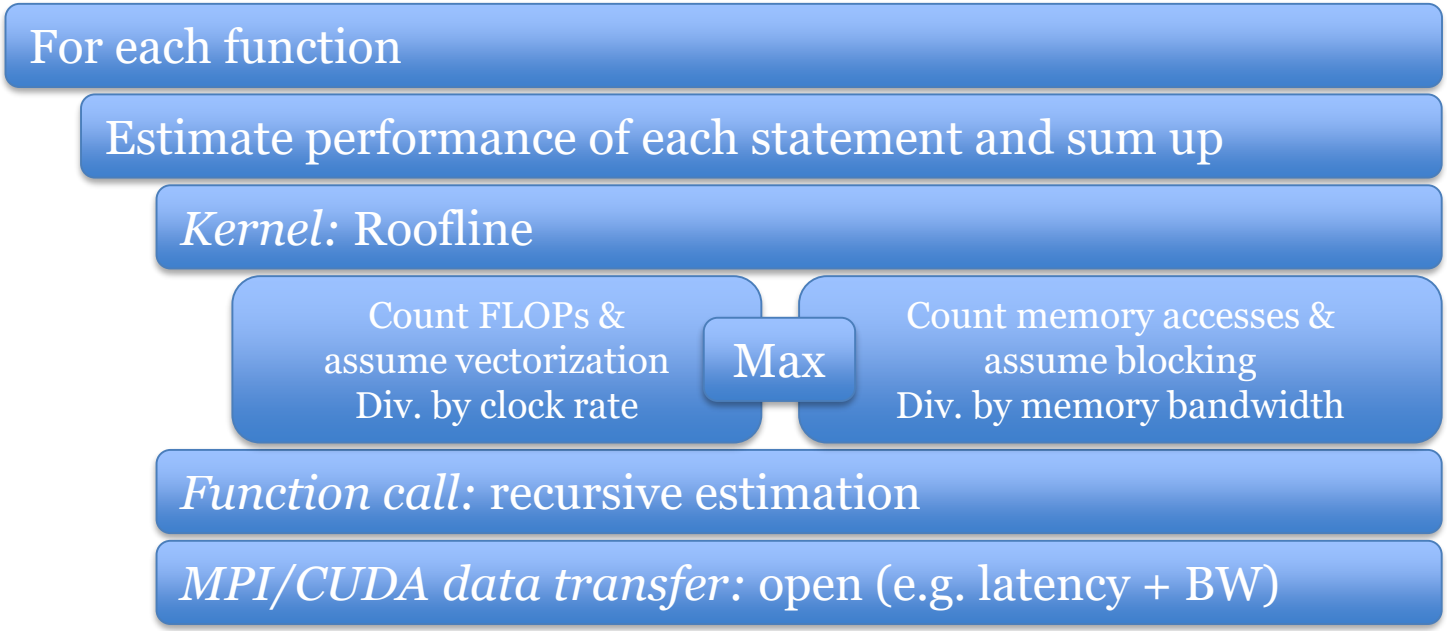
Performance Model: Runtime Prediction



Gmeiner, Köstler et al, *Parallel multigrid on hierarchical hybrid grids: a performance study on current high performance computing clusters*, Concurrency and Comp.: Practice and Experience, 2012.

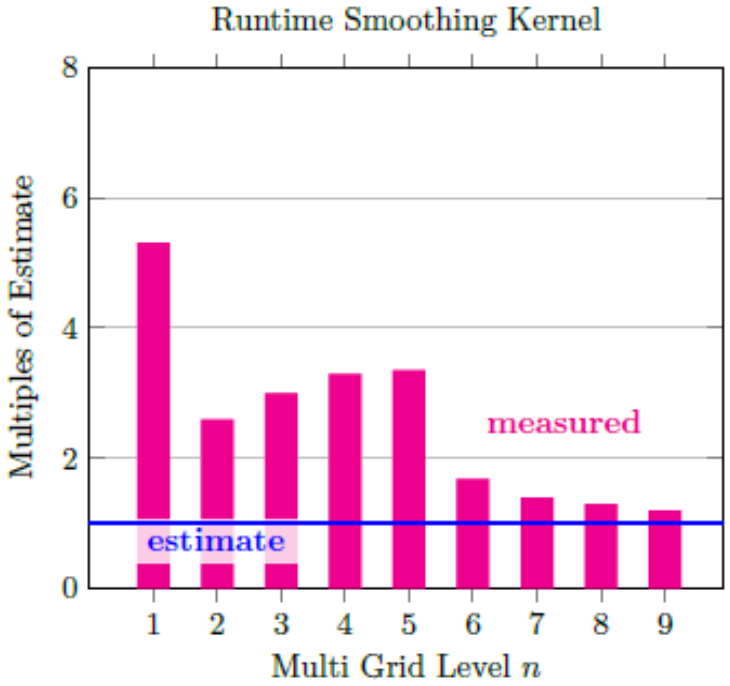
Performance Modeling

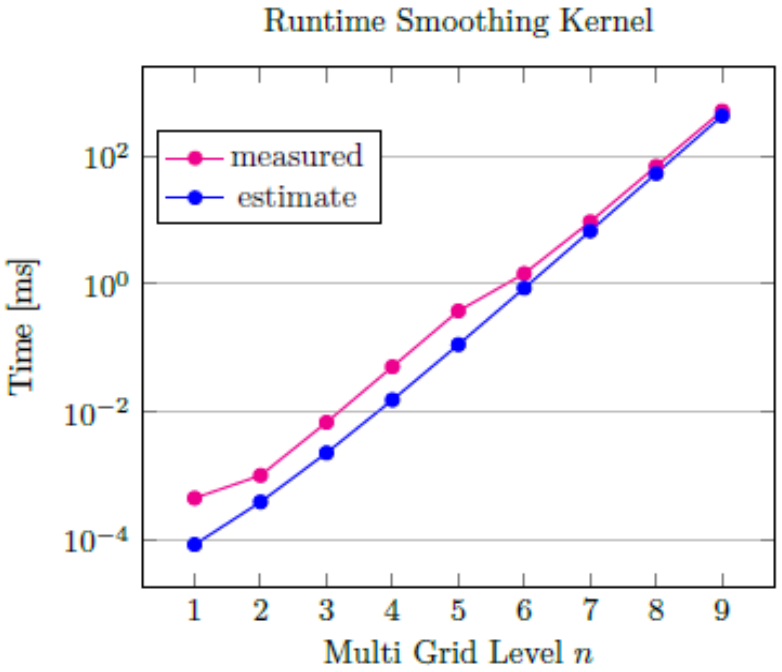
- We aim for an automatic derivation of performance models
- Prototype implementation (optimistic):

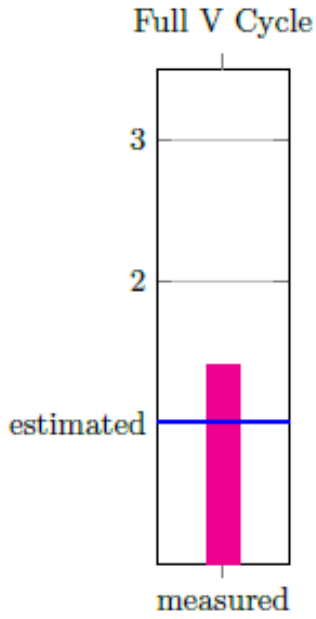


- Ongoing work: extension to ECM

Runtimes 3D Variable Coefficients







CPU dual socket Xeon E5620, 2.4 GHz clock, 4 cores / 8 hw-threads
Microarchitecture Westmere-EP/Gulftown (2010)
L3 Cache 12 MB smart cache
Main Memory 24 GB
Interconnect 2x QPI 5.86 GT/s

Towards Metaprogramming

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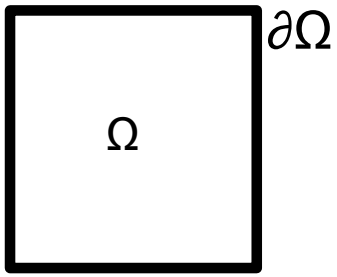
What is the problem?

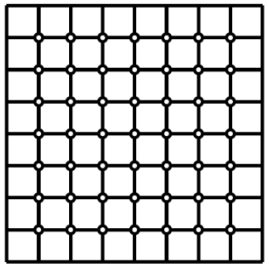
- Goal: Solve partial differential equation

$$\Delta u = f \quad in\ \Omega$$
$$u = 0 \quad on\ \partial\Omega$$

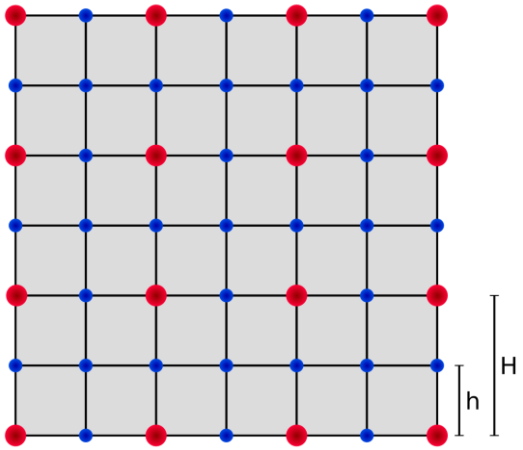


- After discretization one requires an efficient iterative solver for sparse systems

$$Au_h = f_h$$



- Multigrid solver has complexity O(N)



Metaprogramming

Mathematical representation

$$\Delta u = f$$

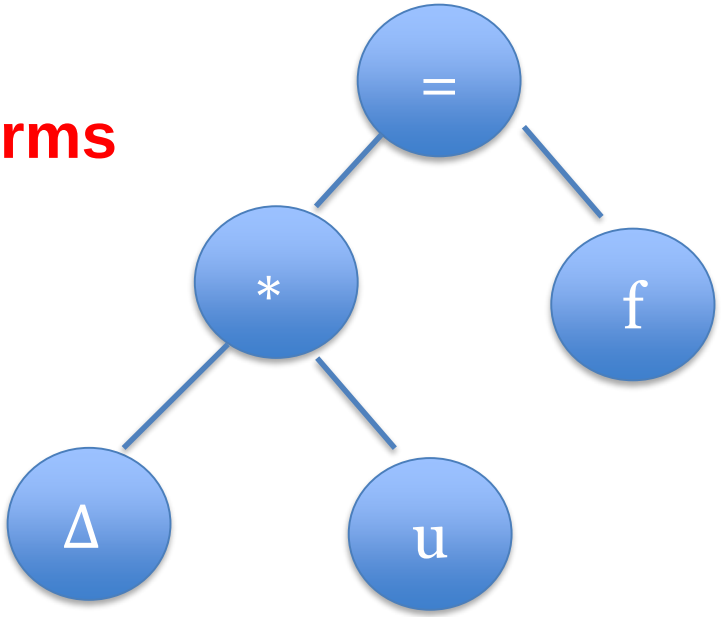
Code representation

```
Field u,f;

Laplace(u) = f;
```

Transforms

Tree representation



Idea: Generate solver automatically

- Linear system of interest as Ax = b, where A is the system matrix, x is the unknown vector and b is the right hand side vector.
- Denote the iteration matrix with M and it is represented as a tree
- The approximated solution in the n+1 iteration is obtained using the old solution and the iteration matrix using the relation $x_{n+1} = Mx_n$.
- A tree in any stage of the framework is a valid expression based on the defined matrix operations i.e. the nodes of the tree are selected such that the generated tree is consistent in terms of dimensions and the generated expressions are secured to be computable.

Genetic Programming Setup

- Terminal Set: It is composed of arbitrary symbolic matrices.
  - **A**, **b**, diagonal of **A**, inverse of the diagonal of **A**, **A** minus its diagonal, lower triangular part of **A**, inverse of the lower triangular part of **A** and upper triangular (1st diagonal) part of **A**.
- Operation Set:
  - The operation set consists of addition, subtraction and multiplication.
- Fitness Evaluation:
  - The symbolic matrix corresponding to the genetic expression of an individual is simplified using the symbolic Math Toolbox of MATLAB and then evaluated to get the numerical version of the iteration matrix.
  - spectral radius r is used to rank individuals, fitness function **f** for $r < 1$ is defined $f(r) = 1/(1- r^2)$ and for $r > 1$ as $f(r) = a_O + a_1 r$

Examples of individuals of iteration matrix

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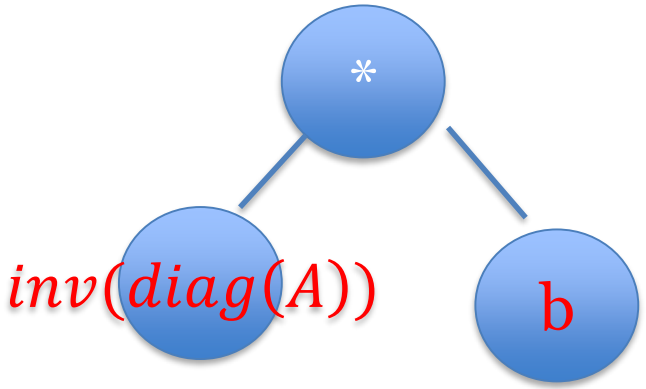
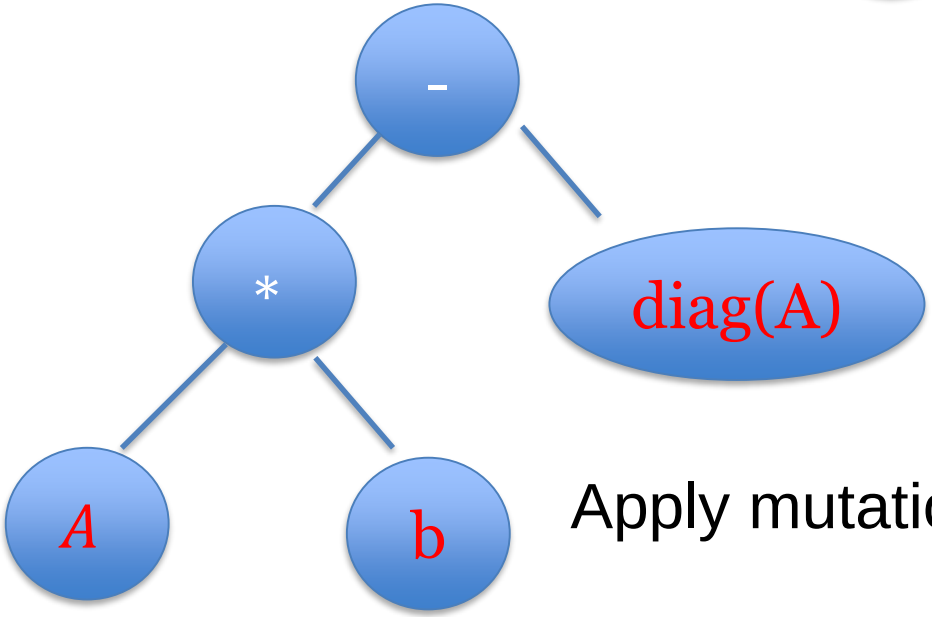
Mathematical representation

M0 = $inv(diag(A)) * b$

M1 = $A * b - diag(A)$

Tree representation

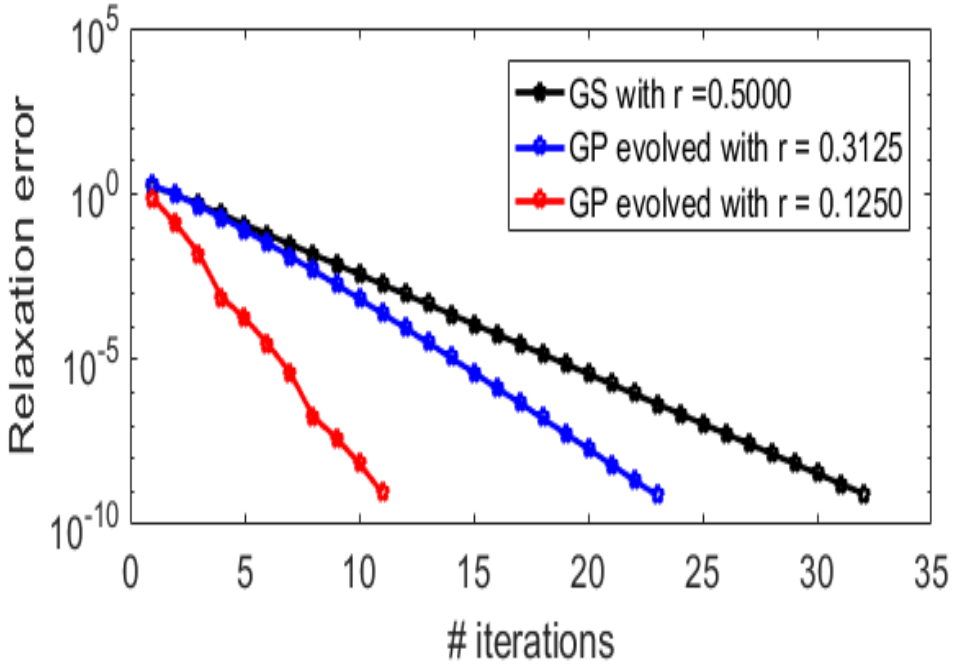




Apply mutation and cross over

1D Example

$$A = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 \end{bmatrix}, b = \begin{bmatrix} 4 \\ 0 \\ -2 \end{bmatrix} \text{ and } x = \begin{bmatrix} 2.5 \\ 1.0 \\ -0.5 \end{bmatrix}$$



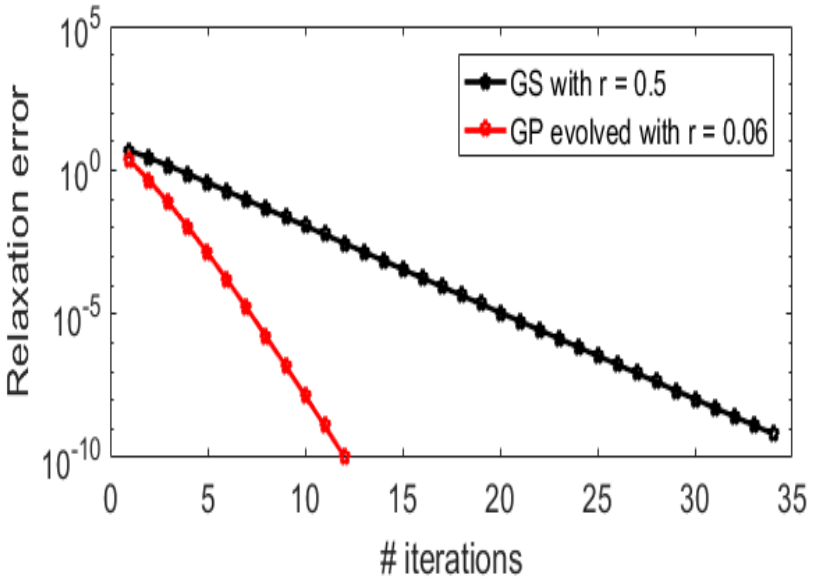
$$M_1 = [\frac{a_{22}a_{33} - a_{11}a_{12}a_{21}a_{33} + a_{11}a_{13}a_{21}a_{32} - a_{11}a_{13}a_{22}a_{31}}{a_{11}^2 a_{22}a_{33}}, \frac{a_{12}a_{33} - a_{13}a_{32}}{a_{11}a_{22}a_{33}}, a_{13}/(a_{11}a_{33})],$$

$$M_2 = [-\frac{a_{23}a_{31}a_{22}^2 - a_{21}a_{23}a_{32}a_{22} + a_{21}a_{33}}{a_{11}a_{22}^3 a_{33}}, \frac{a_{33} - a_{22}a_{23}a_{32}}{a_{22}^3 a_{33}}, \frac{a_{23}}{a_{22}a_{33}}]$$

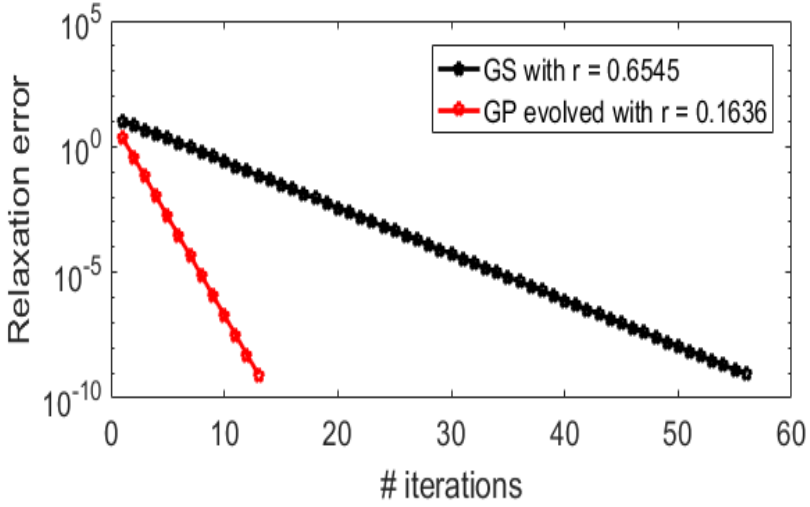
$$M_3 = [\frac{a_{21}a_{32} - a_{22}a_{31}}{a_{11}a_{22}a_{33}^2}, -\frac{a_{32}}{a_{22}a_{33}^2}, \frac{1}{a_{33}^2}]$$

2D Poisson Example

$$A = \begin{bmatrix} 4 & -1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & 0 & -1 \\ 0 & -1 & 4 & 0 & 0 & -1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 4 & -1 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & -1 & 4 & -1 & 0 & -1 & 0 \\ 0 & 0 & -1 & 0 & -1 & 4 & 0 & 0 & -1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 4 \end{bmatrix}$$

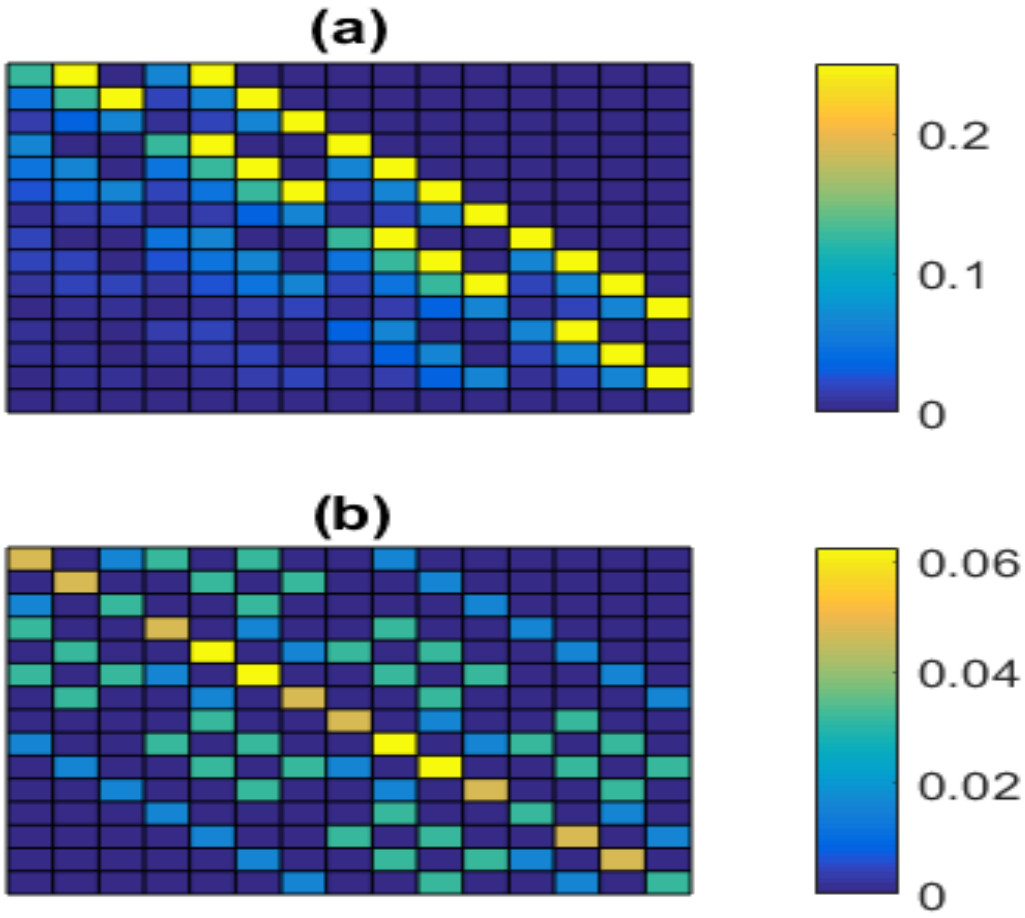


$\boldsymbol{M_1}$ = [-6, 0, 0, 0, 0, 0, 0, 0, 0]e-2 , $\boldsymbol{M_2}$ = [-9, -6, 0, 0, 0, 0, 0, 0, 0]e-2 , $\boldsymbol{M_3}$ = [-3, -9, -6, 0, 0, 0, 0, 0, 0]e-2 , $\boldsymbol{M_4}$ = [-9, 0, 0, -6, 0, 0, 0, 0, 0]e-2 , $\boldsymbol{M_5}$ = [-5, -9, 0, -9, -6, 0, 0, 0, 0]e-2 , $\boldsymbol{M_6}$ = [-2, -5, -9, -2, -9, -6, 0, 0, 0]e-2 , $\boldsymbol{M_7}$ = [-3, 0, 0, -10, 0, 0, -6, 0, 0]e-2 , $\boldsymbol{M_8}$ = [-2, -3, 0, -5, -10, 0, -10, -6, 0]e-2 , $\boldsymbol{M_9}$ = [-1, -2, -3, -2, -5, -10, -3, -10, -6]e-2.



Scalable iteration matrices?!

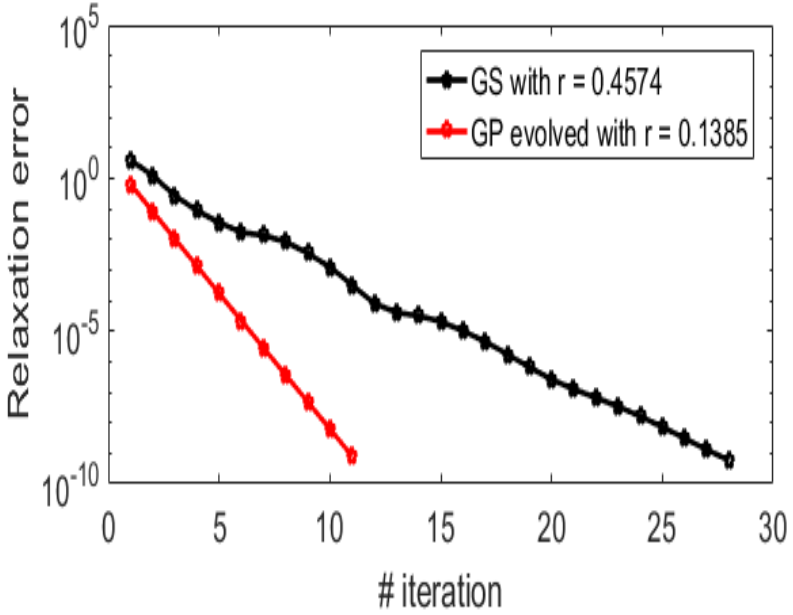
Comparsion of iteration matrices



Optimize pattern for parallelization!

Non-sparse and assymetric system

$\boldsymbol{A_1}$ = [8, 2, 7, 2, 2], $\boldsymbol{A_2}$ = [2, 7, 5, 3, 2], $\boldsymbol{A_3}$ = [3, 4, 8, 3, 3], $\boldsymbol{A_4}$ = [2, 1, 3, 8, 3], $\boldsymbol{A_5}$ = [2, 3, 5, 1, 8] and the column vector $\boldsymbol{b}$ = [105, 108, 100, 56, 82].



$$\boldsymbol{M_1} = \left[\frac{1}{a_{11}}, 0, 0, 0, 0\right], \boldsymbol{M_2} = \left[0, \frac{1}{a_{22}}, 0, 0, \quad 0\right], \boldsymbol{M_3} = \left[0, 0, \frac{1}{a_{33}}, 0, 0\right], \boldsymbol{M_4} = \left[0, 0, 0, \frac{1}{a_{44}}, 0\right], \boldsymbol{M_5} = \left[0, 0, 0, 0, \frac{1}{a_{55}}\right]$$

A simple preconditioner based on inv(A)!

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Thank you for your Attention!

Questions?

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