Automatic Generation of Algorithms and Data Structures for Geometric Multigrid

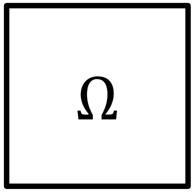
Harald Köstler, Sebastian Kuckuk
Siam Parallel Processing
02/21/2014

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG
TECHNISCHE FAKULTÄT

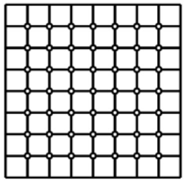
Introduction

Multigrid

- Goal: Solve a partial differential equation approximately by solving a discretized form of said PDE



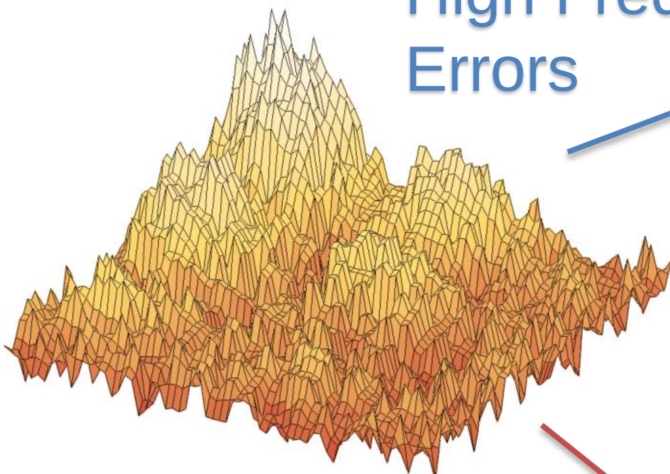
$$\Delta u = f \quad \text{in } \Omega$$
$$u = 0 \quad \text{in } \partial\Omega$$



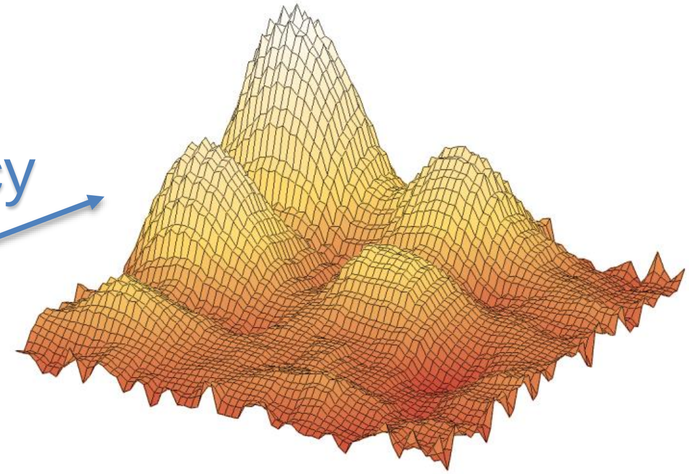
$$A\, u_h = f_h$$

- An efficient method to solve such discretized PDEs in O(N) is multigrid
- Basic idea: Treat high frequency and low frequency errors separately by smoothing and solving for coarse grid representations respectively

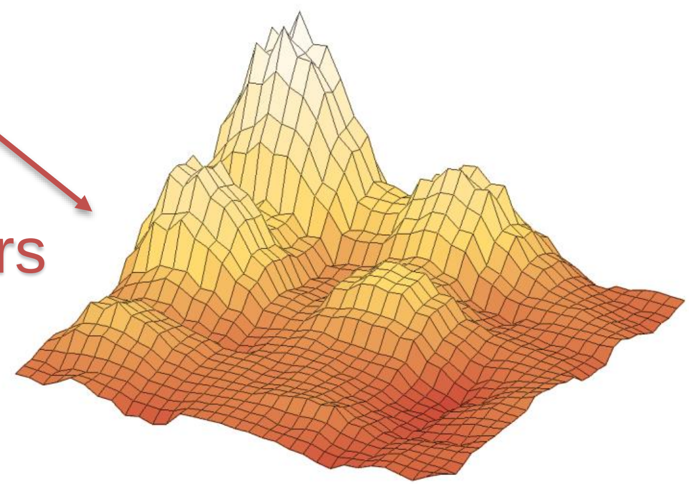
Multigrid



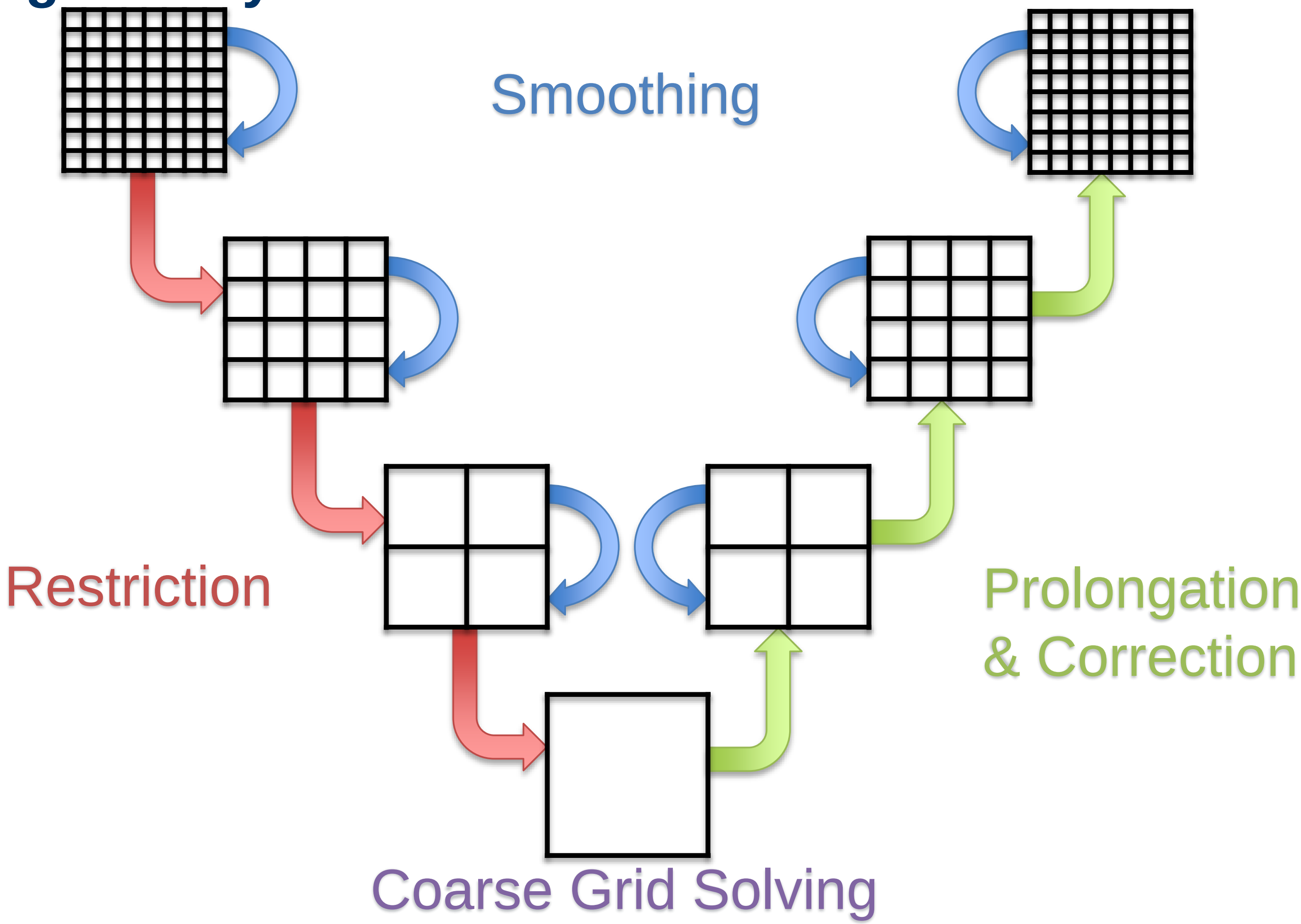
Smoothing of
High Frequency
Errors



Coarsened
Representation of
Low Frequency Errors

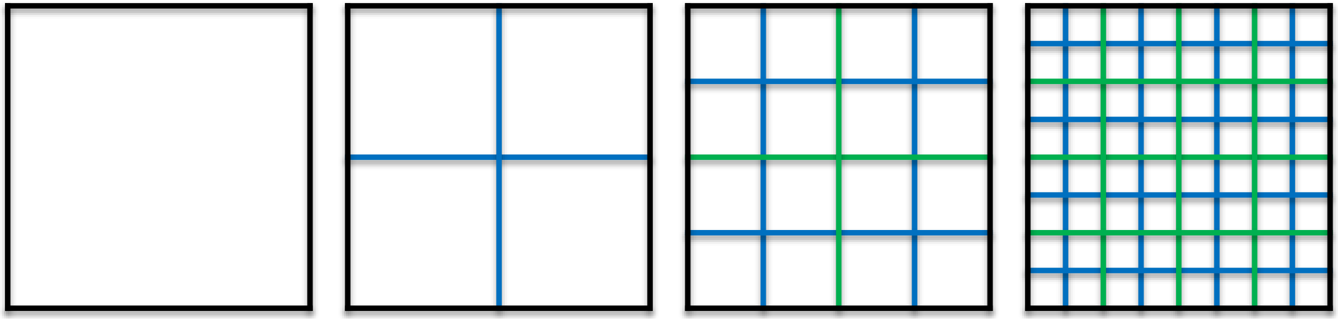


Multigrid V-Cycle

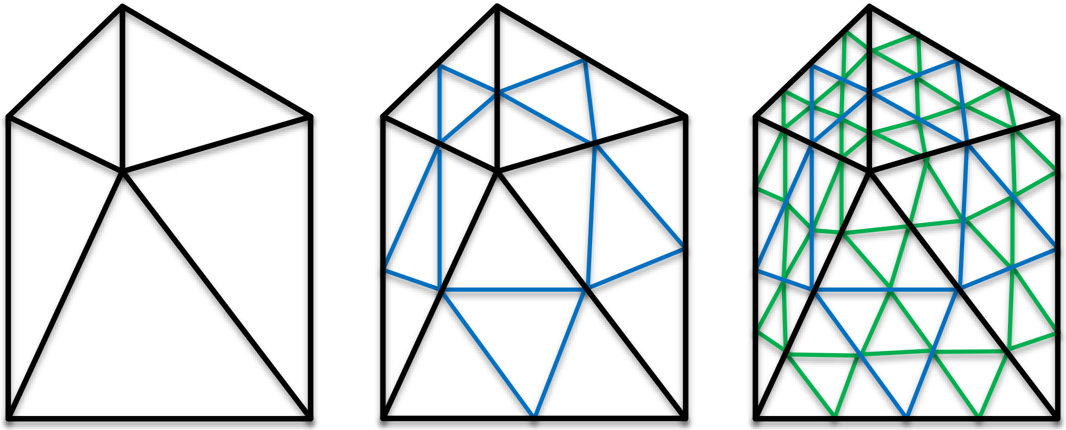


Our Scope

- Uniform grids



- Block-Structured grids



Goals

- What do we want?
  - Efficient and robust multigrid solvers
  - Performance portability
  - Easy to adapt to new settings and concepts (e.g. hardware)
  - Easy to extend
  - …
- Solutions?
  - Extensive Libraries?
  - Optimizing by hand?
  - Auto-Tuning?

Problem – Variance

- There is a lot of variance in the MG domain:
  - Hardware: CPU, GPU or both? Number of nodes, sockets and cores? Cache characteristics? Network characteristics?
  - Software: MPI, OpenMP or both? CUDA or OpenCL? Which version?
  - MG components: Cycle Type? Which smoother(s)? Which coarse grid solver? Which inter-Grid operators?
  - MG parameters: Relaxation? Number of smoothing steps? Other component dependent parameters?
  - Optimizations: Vectorization? (Software) Prefetching? Tiling? Temporal Blocking? Loop transformations?
  - Problem description: Which PDE? Which boundary conditions?
  - Discretization: Finite Differences, Finite Elements or Finite Volumes?
  - Domain: Uniform or block-structured? How to partition?
  - …

Possible Solutions

- What do we want?
  - Efficient and robust multigrid solvers
  - Performance portability
  - Easy to adapt to new hardware
  - Easy to extend
  - …
- Solutions?
  - Extensive Libraries?
  - Optimizing by hand?
  - Auto-Tuning?
  - Code generation?

The ExaStencils Project

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

TECHNISCHE FAKULTÄT

Project ExaStencils

- Sebastian Kuckuk
- Harald Köstler
- Ulrich Rüde

Software Product-Line Group

- Alexander Grebhahn
- Sven Apel

SPPEXA

ExaStencils

- Christian Schmitt
- Frank Hannig
- Jürgen Teich

- Hendrik Rittich
- Matthias Bolten

- Stefan Kronawitter
- Armin Größlinger
- Christian Lengauer

FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG

BERGISCHE UNIVERSITÄT WUPPERTAL

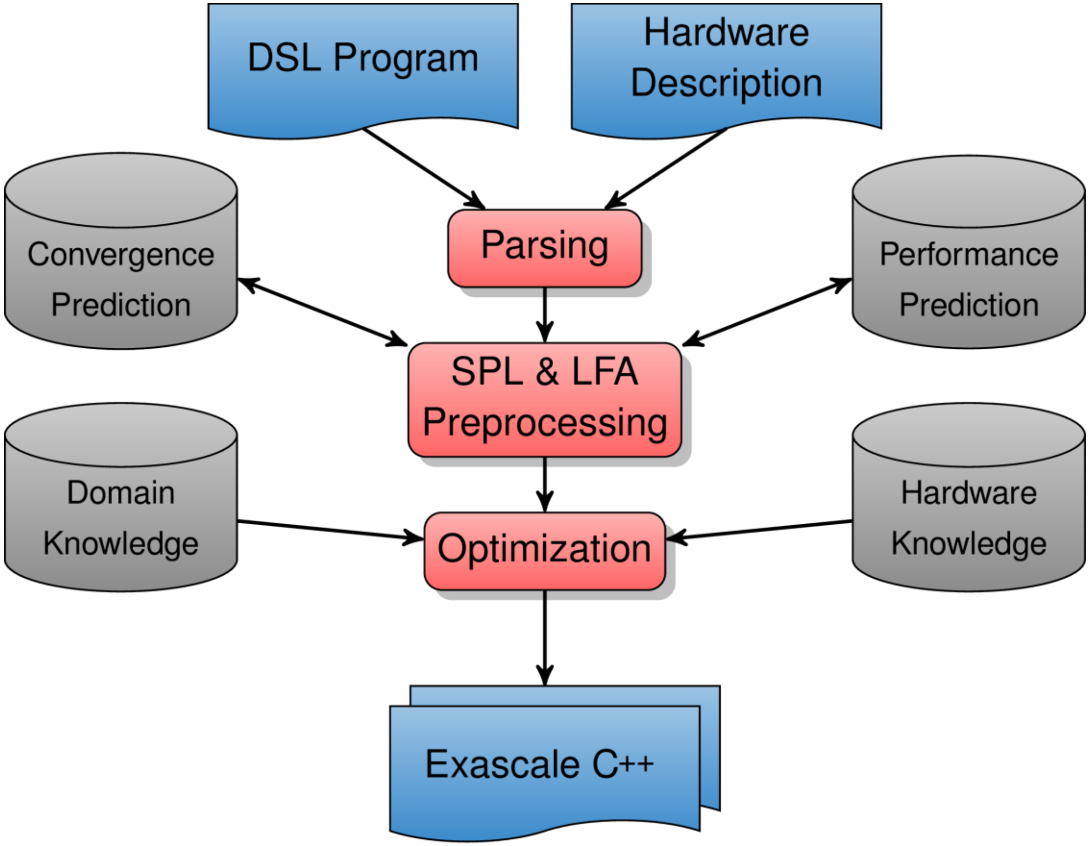
UNIVERSITÄT PASSAU

ExaStencils Vision

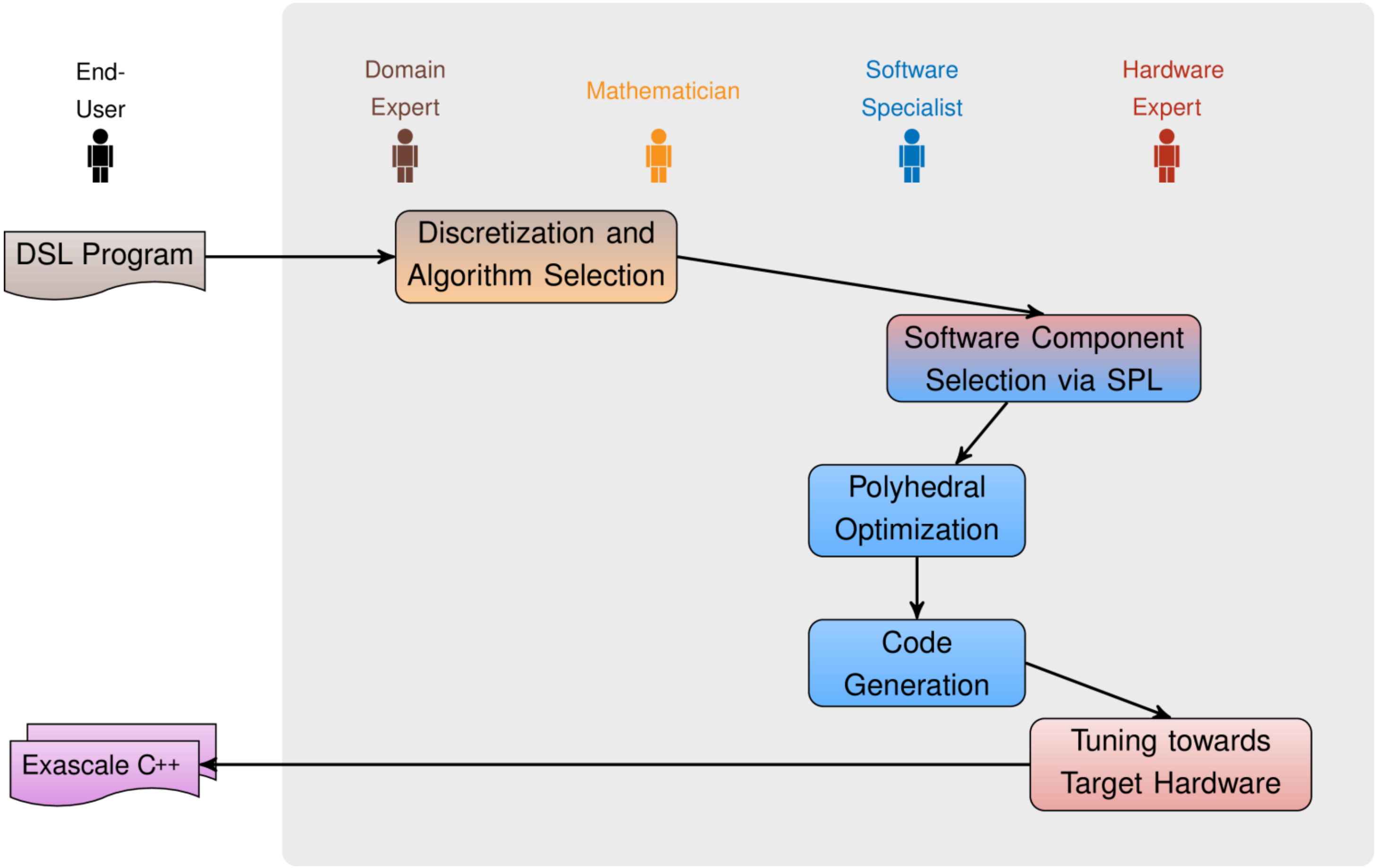
- Generate exa-scalable C++ code for GMG solvers from
  - a high-level problem description specified by domain experts and
  - a target hardware architecture specification

ExaStencils Overview

- DSL as intuitive interface to the user
- Automatic deduction of configuration if desired
- Prediction and Optimization of the configuration's performance using SPL and LFA
- Code generation in Scala
- Automatic hardware-specific optimizations



ExaStencils Workflow



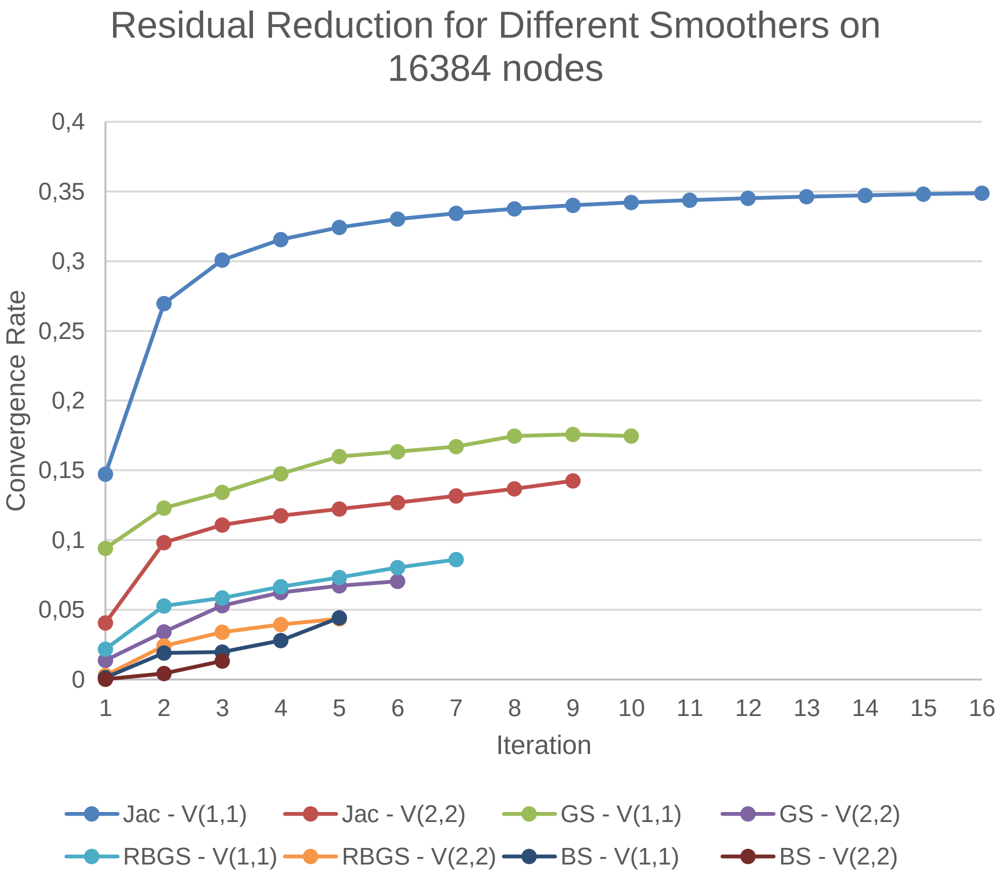
ExaStencils Vision

- Generate exa-scalable C++ code from
  - a high-level problem description specified by domain experts and
  - a target hardware architecture specification
- Further visions: Provide different levels of abstraction that can be used as testing environments for
  - Mathematicians researching multigrid methods and components
  - Software Specialists researching programming languages, efficient communication strategies and program optimizations
  - Hardware Experts researching low-level and hardware-specific optimizations

State of the Project

Current State – LFA

- Convergence rate prediction for 2D/3D Jacobi, Gauss-Seidel, Red-Black Gauss-Seidel
- Hybrid GS and RBGS are predictable for small blocks as well
- Supports all cycle types

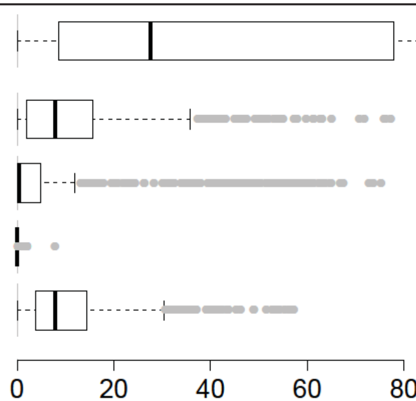


FRIEDRICH-ALEXANDER UNIVERSITÄT ERLANGEN-NÜRNBERG
TECHNISCHE FAKULTÄT

Current State – SPL

- First experiments in applying SPL techniques to our domain have been conducted [2]

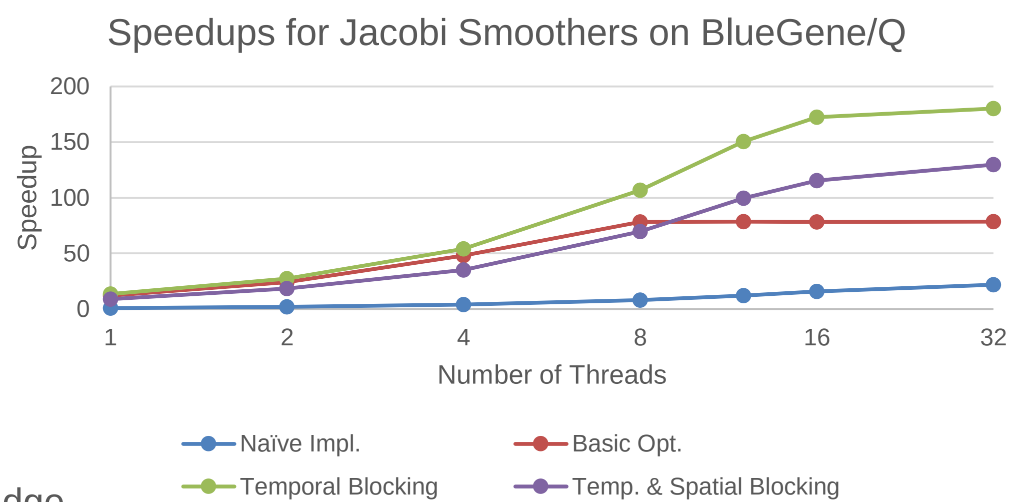
Heuristic	# M	# M [%]	Time [ms]	Faultrate distribution	$\mu \pm \sigma$ [%]	Δ [ms]	δ [%]
FW	22	2.5	51 773.21		51.9 ± 59.3	93.81	8.3
PW	192	22.2	518 721.48		12.2 ± 14.7	184.80	16.3
HO	636	73.6	2 037 253.25		8.5 ± 17	2474.11	217.5
HS	864	100.0	2 230 326.94		0.2 ± 0.6	5.06	0.4
FL	88	10.2	209 415.50		11.2 ± 10.9	695.31	61.1
BF	864	100.0	2 230 326.94		—	—	—

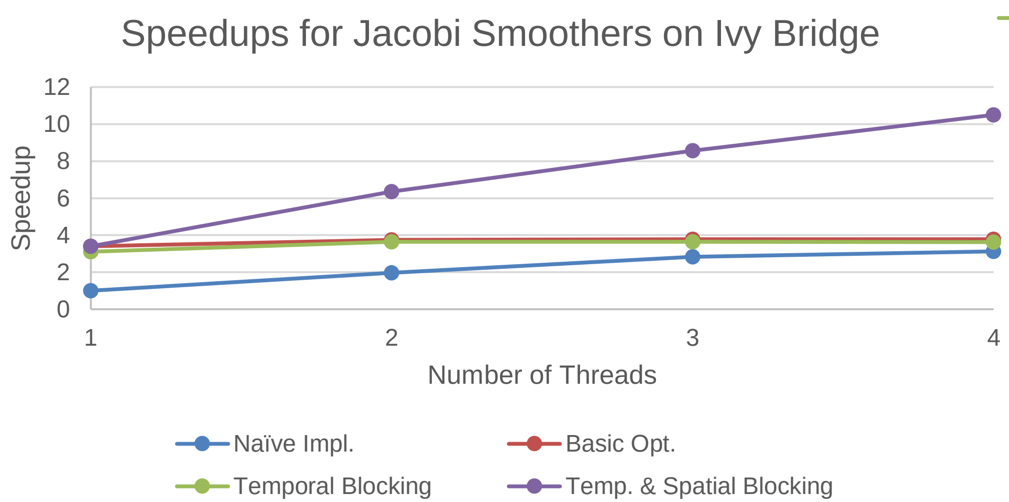


FW: feature-wise, PW: pair-wise, HO: higher-order, HS: hot-spot, FL: function learning, BF: brute force, # M: number of measurements required for the heuristic, Time: runtime for all measurements neglecting compilation times, μ: average error rate, σ: standard deviation, Δ: absolute difference between the measured performance of the optimal configuration and the measured performance of the configuration predicted to perform best, δ: percentage share of Δ on measured performance of the optimal configuration.

Current State – HW Optimizations

- Experiments with basic optimizations (vectorization, address pre-calculation) and temporal/ spatial blocking on different hardware architectures [3]



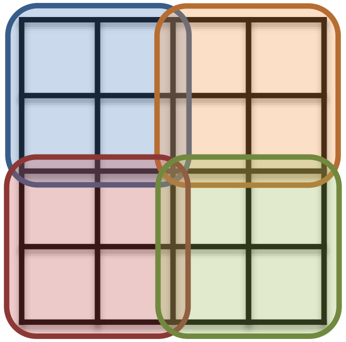


Current State – DSL(s)

- Different levels
  1. Continuous model (PDE, Domain)
  2. Discrete model (Stencils, Fields)
  3. Algorithmic components & parameters
  4. Pseudo-code for critical functions
- Prototype DSLs for each level
- First work on deriving levels from previous configurations

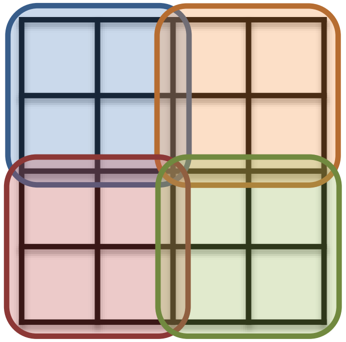
Current State – Code Generation (Multigrid)

- Multigrid
  - Scala prototype capable of generating fully working multigrid solvers for FD discretizations of Poisson's equation in 2D and 3D
- Domain Generation
  - Currently only uniform grids, i.e. no HHG (Hierarchical Hybrid Grids) data structures
  - Domain is divided into rectangular blocks
  - Each block is composed of one or more fragments
  - Domain is setup at runtime
  - This includes memory for data fields, neighborhood connections, temporary memory for communication, …



Current State – Code Generation

- Parallelization
  - Uniform grids in 2D or 3D
  - Different communication schemes (6P/26P in 3D and 4P/8P in 2D)
  - Pure MPI or hybrid OpenMP-MPI parallelization
  - OpenMP parallelization by replacing MPI communication with local communication or by agglomeration of fragments and parallelizing the stencil kernels directly
  - Optional usage of MPI data types for sending and receiving field data in most cases
  - Variable number of ghost layers
  - …

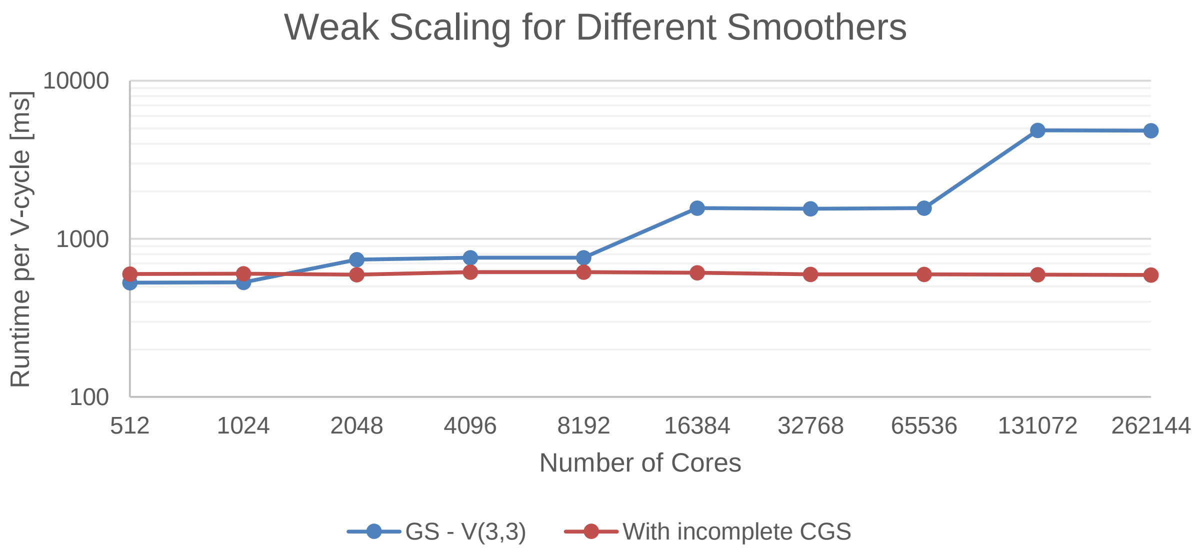


JuQueen

- 28 672 Nodes (458 752 Cores)
- Compute Node: IBM PowerPC A2, 1.6 GHz, 16+1+1 cores
- Main memory:
  16 GB per node
  (aggregate 448 TB)
- Overall peak performance:
  5.9 PetaFLOP/s

(Very) Preliminary Results for 3D FD Poisson

- Weak scaling for a V(3,3) cycle with Gauss-Seidel as smoother
- Coarse-grid solver is not implemented yet; thus, we use the smoother as CGS with the number of iterations according to
  a) the squared maximum of the number of fragments per dimension or
  b) a fixed number of iterations

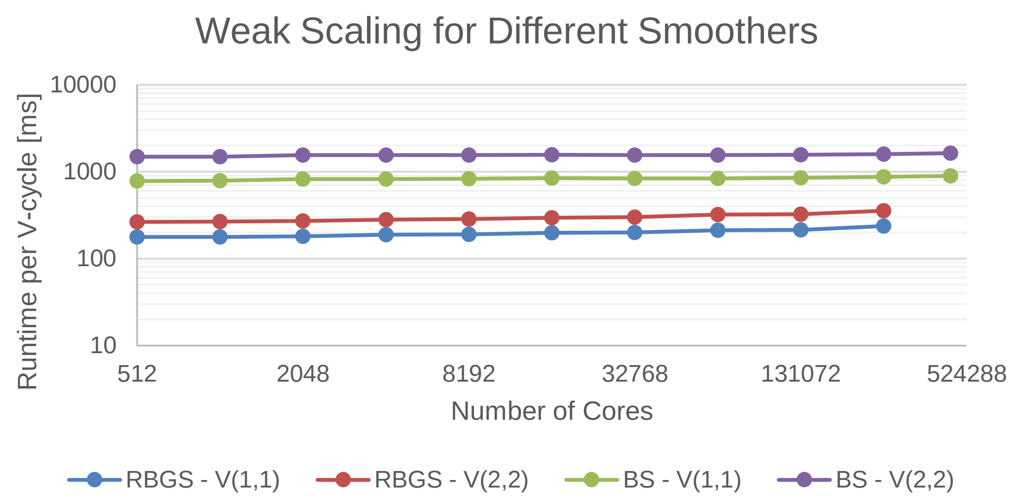


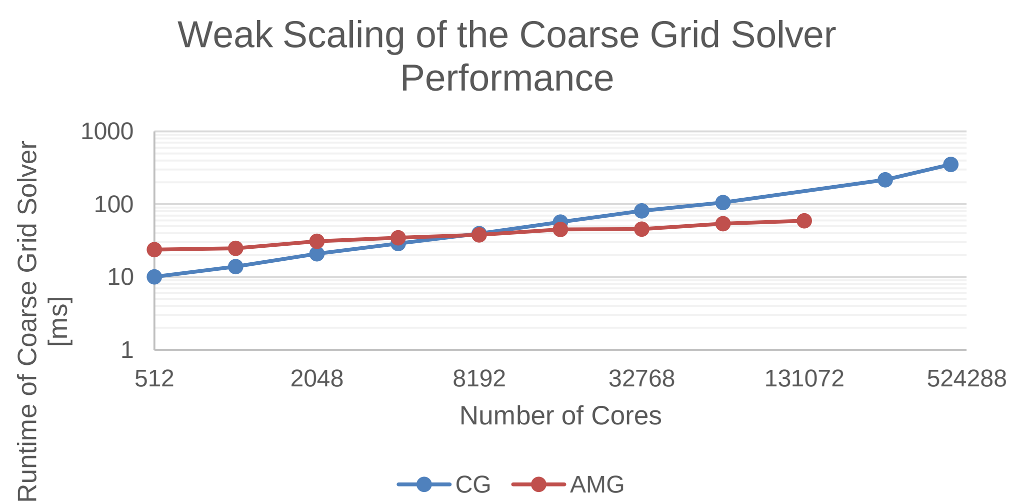
Next Steps

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG
TECHNISCHE FAKULTÄT

Next Steps

- Multigrid
  - Integrate missing multigrid components to allow for comparison with our old multigrid codes [1]
  - This mainly includes coarse-grid solvers
- Data structures
  - Generate HHG data structures and the necessary stencil application codes





Next Steps

- Low-level optimization
  - Setup an interface between the code generator and the polyhedron model
  - Express transformations in polyhedron model
- Runtime prediction and optimization (LFA & SPL)
  - Develop a more precise model for feature interactions
  - Extend the LFA tool
  - Combine the two approaches to yield an efficient and robust optimization

References

(1) Sebastian Kuckuk, Björn Gmeiner, Harald Köstler, and Ulrich Rüde. *A generic prototype to benchmark algorithms and data structures for hierarchical hybrid grids.* Accepted at ParCo2013.

(2) Alexander Grebhahn, Norbert Siegmund, Sven Apel, Sebastian Kuckuk, Christian Schmitt, and Harald Köstler. *Optimizing Performance of Stencil Code with SPL Conqueror.* In Proceedings of the 1st International Workshop on High-Performance Stencil Computations (HiStencils), pages 7–14, January 2014.

(3) Stefan Kronawitter and Christian Lengauer. *Optimization of two Jacobi Smoother Kernels by Domain-Specific Program Transformation.* In Proceedings of the 1st International Workshop on High-Performance Stencil Computations (HiStencils), pages 75–80, January 2014.

Thank you for your Attention!

Questions?

FRIEDRICH-ALEXANDER
UNIVERSITÄT
ERLANGEN-NÜRNBERG

TECHNISCHE FAKULTÄT