Towards a Parallel Algebraic Multigrid Solver Using PGAS

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Acknowledgment

The main goal of the EC Horizon 2020 funded ExaFLOW project is to address key algorithmic challenges in CFD to enable simulation at exascale,

- Accurate **error control**, adaptive mesh refinement
- Solver **efficiency**, scalable numerical methods and preconditioners
- Strategies to ensure **fault tolerance** and resilience
- **Input/output** for extreme data, data reduction
- **Energy awareness** in solver design

http://www.exaflow-project.eu

Introduction

Why use PGAS languages?

- One-sided communication
- Allow for fine grained parallelism
- More productive languages

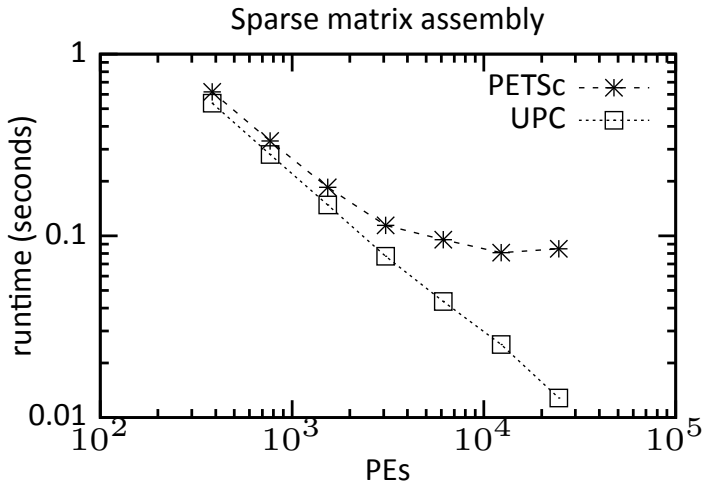
A typical two-sided distributed memory program

Data decomposition
while not done **do**
  Compute local part
  Send/Receive overlap
  Add contribution from overlap
end while

One sided comm. allows for novel parallelization algorithms

PGAS based Linear Algebra library

- Row wise distribution of matrices and column vectors
- Matrix/vector entries accessible by all
  - Easier to write solvers/preconditioners
  - Less synchronization points
- Implemented in Unified Parallel C
- Hybrid interface for use with MPI codes
- Low latency communication kernels
  - Reduce overhead cf. message passing
  - Improving fine grained parallelism
    - Sparse matrix assembly (FEM)
    - Allowing for less elements/core

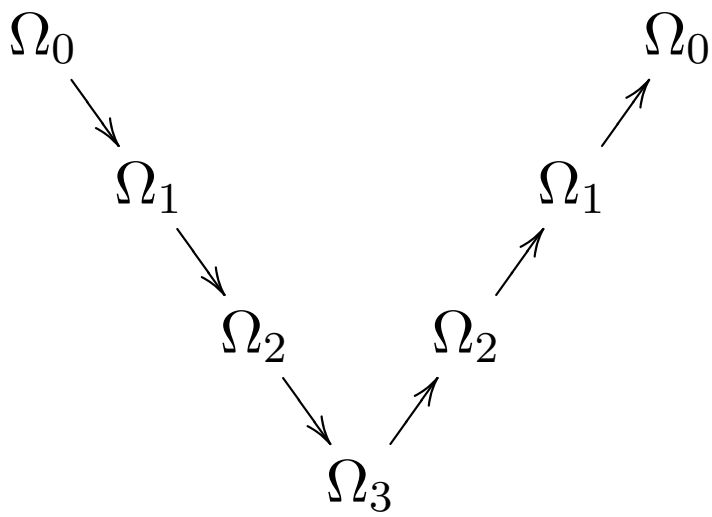


Algebraic Multigrid

A multilevel method for solving $Ax = b$, where A is an $n \times n$ matrix with entries a_{ij} and x, b are vectors of size n.

- Eliminated smooth errors by solving $Ae = r$, on a coarser problem
- Interpolate back, and correct the fine solution, $x = x + e$

if $k =$ coarsest level **then**
  Solve $A^k x^k = f^k$
else
  Relax μ_1 times on $A^k x^k = f^k$
  Set $x^{k+1} = 0$, $f^{k+1} = I_k^{k+1}(f^k - A^k x^k)$
  Apply V--cycle on level $k + 1$
  Correct the solution by
  $x^k = x^k + I_{k+1}^k x^{k+1}$
  Relax μ_2 times on $A^k x^k = f^k$
end if



- Asymptotically optimal complexity
- Notorious difficult to parallelize in an optimal way!

AMG coarsening

Let Ω^k be the set of components of x at level k

- Split Ω^k into two disjoint sets C and F
- No underlying geometry
- Need to pick coefficients in A^{k+1} related to a error freq.
- Classify if unknowns are strongly coupled to each other

$$-a_{ij} \geq \theta \max_{k \neq i} \{-a_{ik}\}$$

- Measure λ_i, number of points strongly influenced by i

Ruge-Stüben Coarsening

Related to interpolation quality

> ***C1:*** *For each point j that strongly influences a F-point i, j is either a C-point or it strongly depends on a C-point l that also strongly influences i.*

Size of the coarser level

> ***C2:*** *C should be a maximal subset of all points with the property that no two C points are strongly connected to each other.*

Ruge-Stüben Coarsening

Let $U = \Omega^k$
/* First phase */
while $U \neq \emptyset$ **do**
    Pick an $i \in U$ with maximal λ_i
    Set $U = U - \{i\}$, $C = C + \{i\}$
    Add all points j which strongly depends on i to F
    Increase the measure λ_l for all points l that are strongly dependent on j
    Decrease the measure λ_m for all points m that are strongly dependent on i
end while

/* Second phase */
for all $i \in F$ **do**
    if i violates criteria **C1 then**
        $F = F - \{i\}$, $C = C + \{i\}$
    end if
end for

AMG Coarsening

A challenge for message passing is the restricted local view of the data

- A thread must be able to determine if a neighboring point is *C* or *F*
- Points will change between *F* and *C* during coarsening
- Explicit communication with neighbors
- Less optimal coarsening algorithms
  - Easier parallelization
  - Pay with more multigrid cycles
  - Set/Graph based (CLJP, PMIS HMIS)
  - Heuristics (RS3)

Restrictions comes from a two-sided message passing perspective

- Put *C*/*F* data in global memory
- Accessible by all threads
- Solves most of the parallelization issues

AMG Coarsening

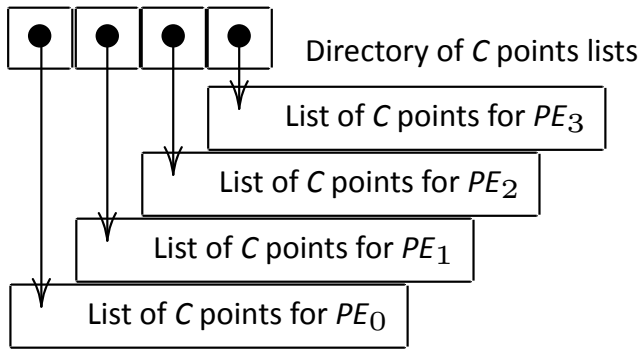
PGAS based RS

Most of the data structures are local

- Unordered set of *C* and *F* points
- Measure λ_i stored in red-black trees

Keep a list of *C* variables in global memory

- PE dependent block size
- Directory approach (arbitrary size)
- Protect the list with a set of variables
  - Declared as UPC `strict`
  - Less expensive than using locks



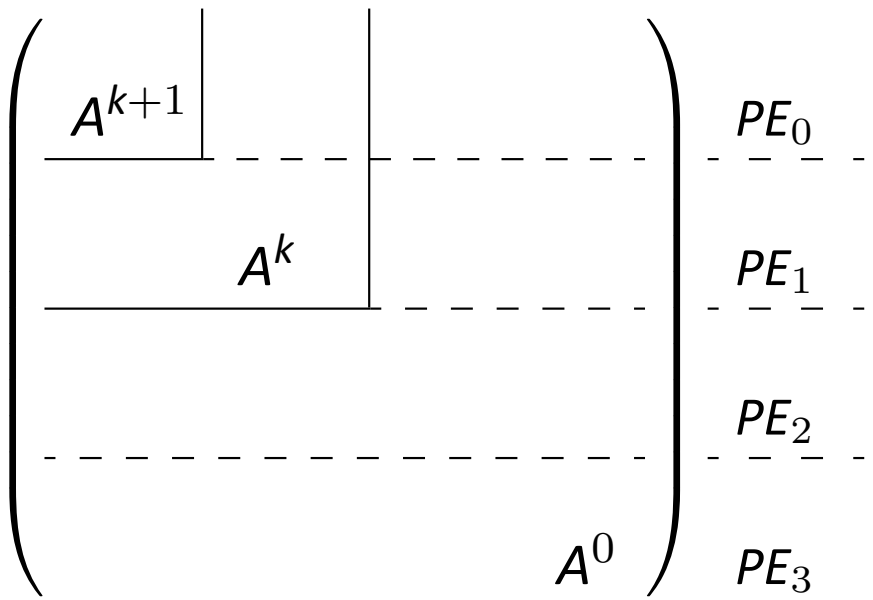
PGAS based RS

Let $U = \Omega^k$ and $Cg(:) = 0$
/* First phase */
while $U \neq \emptyset$ **do**
    Pick an $i \in U$ with maximal λ_i
    Set $U = U - \{i\}$, $C = C + \{i\}$ and $Cg(i) = 1$
    Add all points j which strongly depends on i to F
    Increase the measure λ_l for all points l that are strongly dependent on j
    Decrease the measure λ_m for all points m that are strongly dependent on i
end while
Barrier
/* Second phase */
for all $i \in F$ **do**
    if i violates criteria **C1 then**
        Wait **while** $S(i) \neq 0$
        $S(i) = 1$ /* Protect variable i */
        $F = F - \{i\}$, $C = C + \{i\}$ and $Cg(i) = 1$
        $S(i) = 0$ /* Release variable i */
    end if
end for

Load Balancing

- A^{k+1} becomes smaller and smaller for each coarsening level k
- Move operator towards a single core (easier coarse level solve)
- Use a load balanced linear distribution $N = PL + R$,

$$L = \left\lfloor \frac{N}{P} \right\rfloor,$$
$$R = N \bmod P,$$
$$n = \left\lfloor \frac{N + P - p - 1}{P} \right\rfloor$$



AMG Solver

- Multigrid Cycling
  - Matrix vector products
  - Redistribution routines (load balancing)
- Coarse Level Solver
  - Direct solver (single PE)
  - Krylov solver (multiple PEs)
- Smoother
  - Hybrid *CF* Gauss Seidel

$$x_i^k = \left(b_i - \sum_{j<i} a_{ij} x_j^k - \sum_{j>i} a_{ij} x_j^{k-1} \right) \Big/ a_{ii}$$

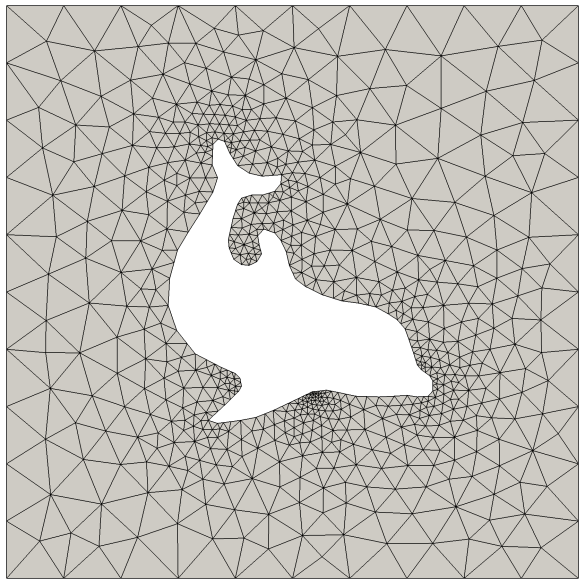
  - Straightforward implementation (PGAS)
  - Work across PE boundaries

Benchmark Problem

Poisson's equation on the unit square

$$
\begin{aligned}
-\Delta u(x,y) &= f(x,y), && (x,y) \in \Omega, \\
u(x,y) &= 0, && (x,y) \in \Gamma_0, \\
\partial_n u(x,y) &= g(x,y), && (x,y) \in \Gamma_1, \\
\partial_n u(x,y) &= 0, && (x,y) \in \partial\Omega \setminus (\Gamma_0 \cup \Gamma_1),
\end{aligned}
$$

$$
\begin{aligned}
f(x,y) &= 500 \exp(-((x-0.5)^2 + (y-0.5)^2)/0.02) \\
g(x,y) &= 25 \sin(5\pi y).
\end{aligned}
$$



Evaluation

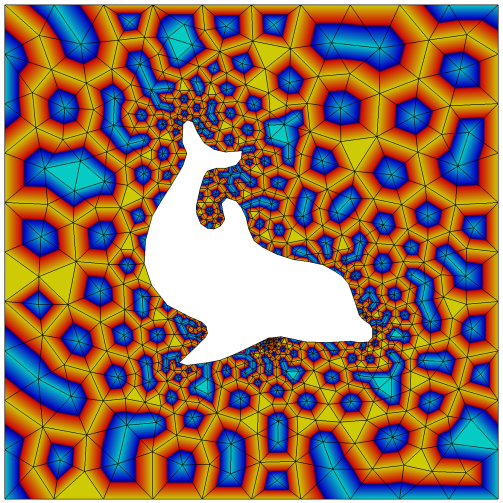
Benchmark Problem

- Discretize PDE by FEM
- Use the FEM framework FEniCS
  - FEniCS assembles the stiffness matrix
  - Linear system solved by external libraries
- Hybrid MPI + PGAS
- Use PETSc as a reference krylov solver
- All experiments performed on the Cray XC40 Beskow at PDC/KTH

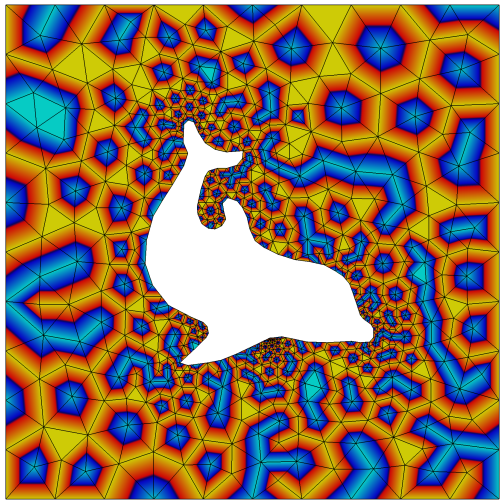
Coarsening Quality

Parallel Coarsening

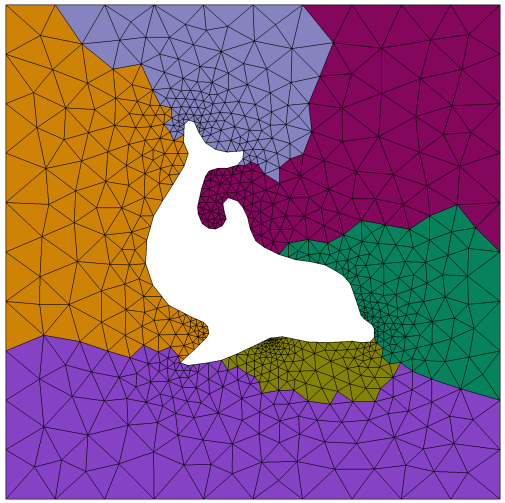
- No artifacts from boundary between partitions



Serial coarsening



Parallel coarsening



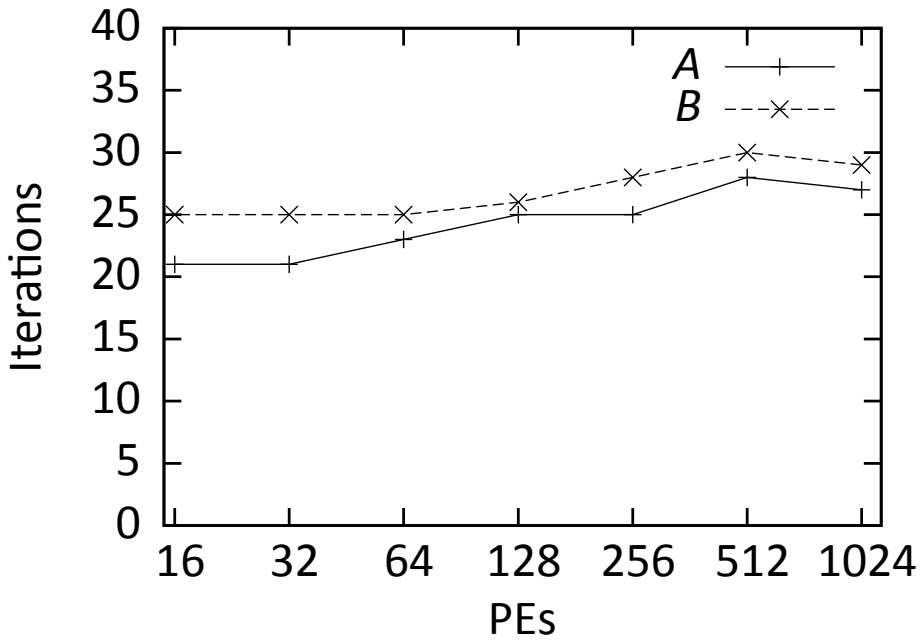
Mesh partitions

Coarsening Quality

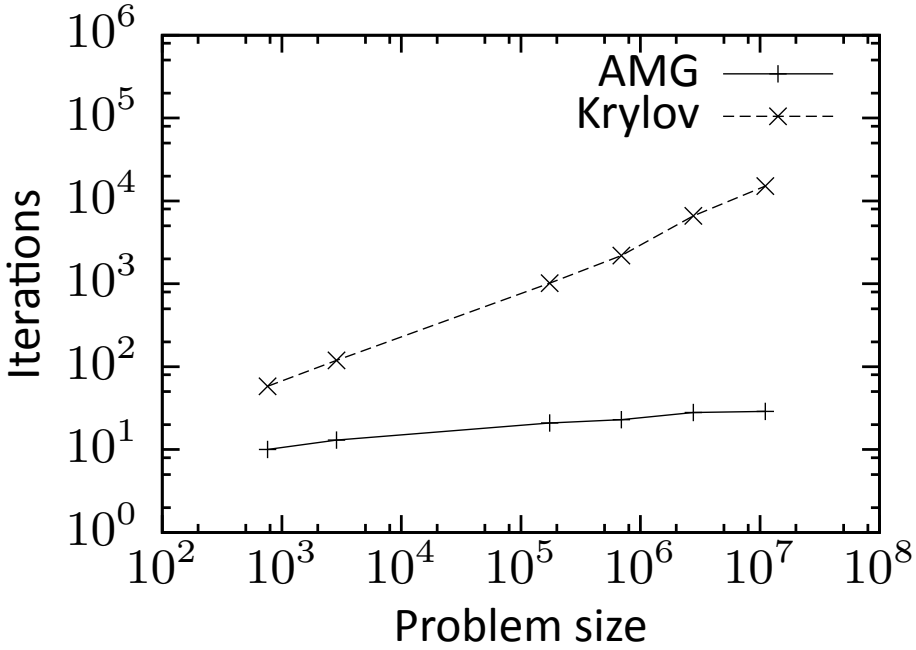
Asymptotically optimal complexity

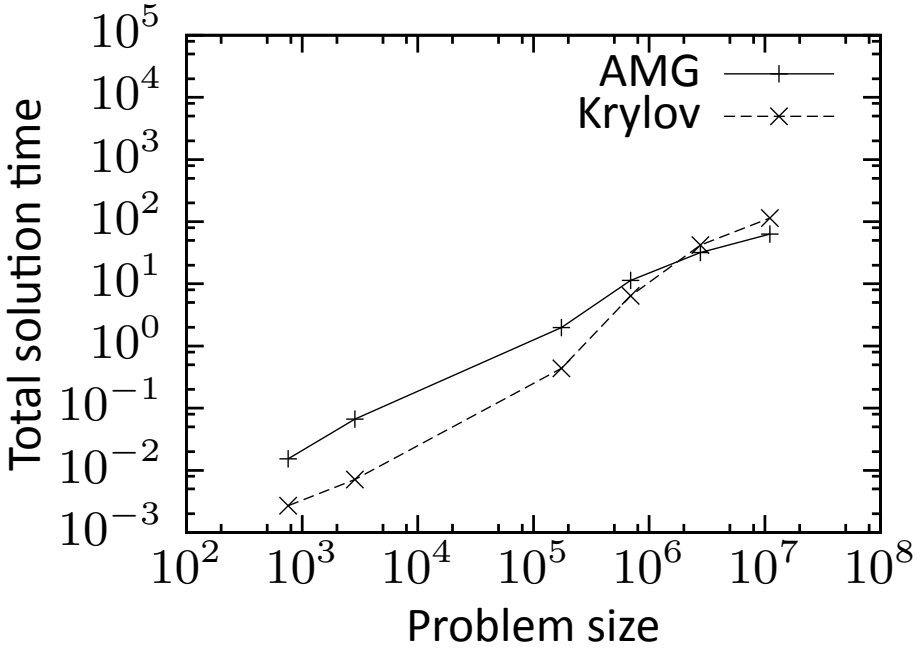
- Number of V-cycles independent of problem size
- Number of V-cycles independent of PEs

Benchmark solved for two matrix sizes and diff. numbers of PEs



Performance





Performance

					AMG				Krylov	
PEs	n	C_{op}	C_{g}	l	Iters	t_{setup}	t_{solve}	t_{tot}	Iters	t_{tot}
1	759	1.821	1.480	2	10	0.008	0.008	0.015	58	0.003
4	2868	2.137	1.552	4	13	0.030	0.037	0.067	119	0.007
32	174144	2.265	1.529	7	21	0.712	1.265	1.977	1023	0.436
128	693888	2.098	1.495	8	23	3.779	7.635	11.414	2196	6.432
512	2770176	2.065	1.486	9	28	8.190	23.601	31.791	6624	42.117
1024	11069952	2.044	1.480	10	29	11.476	51.787	63.263	15139	114.841

- AMG overhead costs too high for small matrices
- AMG setup costs (t_{setup}) less than solve (t_{solve})
- Operator (C_{op}) and grid complexity (C_{g}) doesn't grow
- AMG iterations doesn't grow too much with large numbers of PEs

Summary

- New parallel formulation of Ruge-Stüben
  - Not possible to formulate using MPI
- Retains similar properties as the serial algorithm
- Easier implementation due to the PGAS abstraction

Future work

- Reduce AMG overhead
- Optimized collective operations
  - No subset collectives in std. UPC
  - Handwritten versions not optimized
- Investigate UPC atomics
  - Our Cray compiler didn't support it
  - Alternative instead of strict variables