Optimizing Geometric Multigrid Method Computation using a DSL Approach

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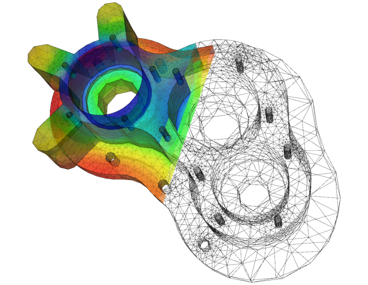
Outline

Iterative Numerical Methods



Visualization of heat transfer in a pump casing; created by solving the heat equation.

- Numerical approximation for partial differential equations
- Approximation is improved every iteration
- Applications in fields of engineering and physical sciences

Multigrid Methods

- **Poisson's equation**

$$\nabla^2 u = f.$$

Multigrid Methods

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- Finite difference discretization; approximate second derivative

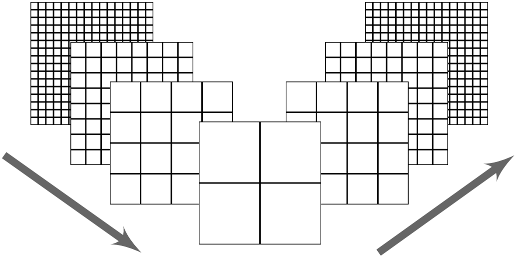
Multigrid Methods

- **Poisson's equation**

$$\nabla^2 u = f.$$

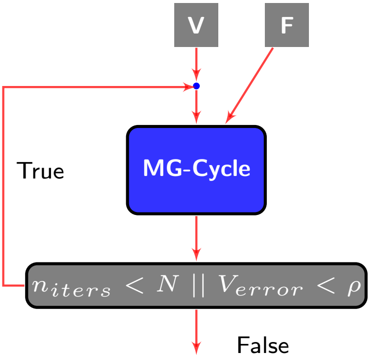
- Finite difference discretization; approximate second derivative
- Solve $f = Au$, where A is a sparse banded matrix (u is a linearization of the unknown on the multi-dimensional grid)
- What about A^{-1}?

Multigrid Methods



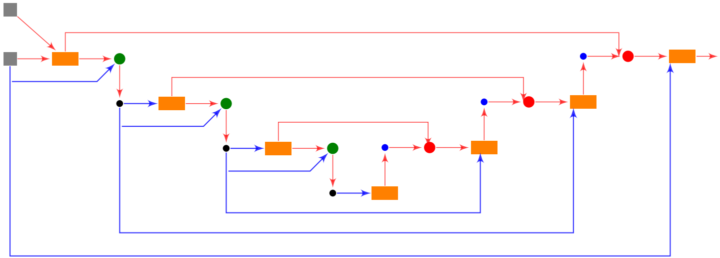
- Involving discretizations at multiple scales
- A fast-forward technique in the iterative solving process
- Used as direct solvers as well as preconditioners

Multigrid Methods



- Unit of execution: multigrid cycle
- Iterate until convergence / for fixed number

Multigrid Cycles: V-Cycle



Smoother

Defect/Residual

Correction

Restrict/Reciprocate

Interpolate/Prolongation

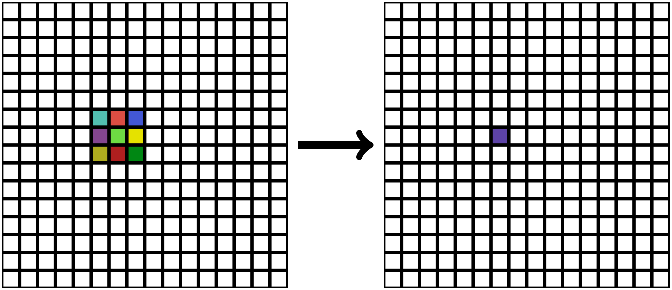
Multigrid Methods

- Heterogeneous composition of basic computations
- Typically expressed as a recursive algorithm
- Optimizations limited to one multigrid cycle

Algorithm 1: V-cycle^h

```
Input : v^h, f^h
Relax v^h for n_1 iterations
// pre-smoothing
if coarsest level then
    Relax v^h for n_2 iterations    // coarse smoothing
r^h ← f^h − A^h v^h                 // residual
r^{2h} ← I_h^{2h} r^h               // restriction
e^{2h} ← 0
e^{2h} ← V-cycle^{2h}(e^{2h}, r^{2h})
e^h ← I_{2h}^h e^{2h}               // interpolation
v^h ← v^h + e^h                     // correction
Relax v^h for n_3 iterations        // post smoothing
return v^h
```

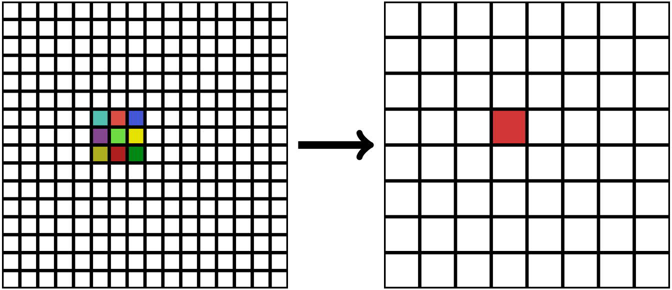
Multigrid Methods: Basic Steps



Smoothing

$$f(x,y) = \sum_{\sigma_x=-1}^{+1} \sum_{\sigma_y=-1}^{+1} g(x+\sigma_x, y+\sigma_y) \cdot w(\sigma_x, \sigma_y)$$

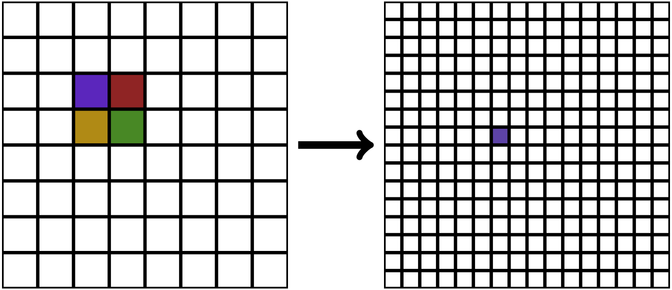
Multigrid Methods: Basic Steps



Restriction/Decimation

$$f(x,y) = \sum_{\sigma_x=-1}^{+1} \sum_{\sigma_y=-1}^{+1} g(2x+\sigma_x, 2y+\sigma_y) \cdot w(\sigma_x, \sigma_y)$$

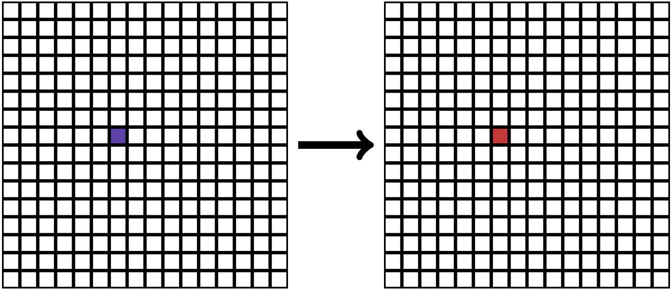
Multigrid Methods: Basic Steps



Interpolation/Prolongation

$$f(x,y) = \sum_{\sigma_x=0}^{+1} \sum_{\sigma_y=0}^{+1} g((x+\sigma_x)/2,(y+\sigma_y)/2) \cdot w(\sigma_x,\sigma_y,x,y)$$

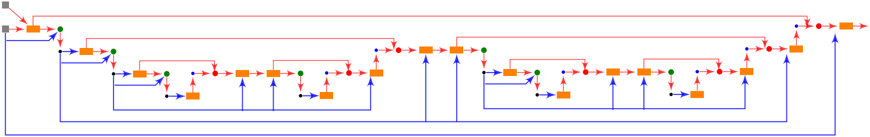
Multigrid Methods: Basic Steps



Point-wise

$$f(x, y) = \alpha \cdot g(x, y)$$

Multigrid Cycles: W-Cycle



Smoother

Defect/Residual

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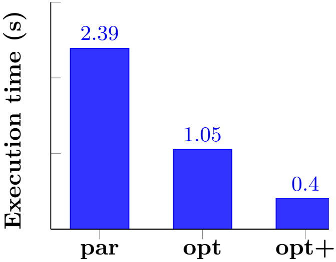
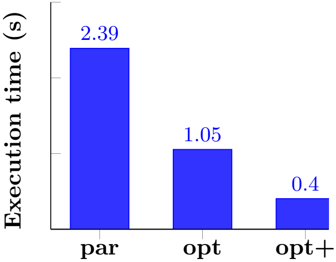
Naive vs Optimized Implementation



Multigrid-2D (Jacobi)
(24 cores)

- Naive parallelization (OpenMP, vector pragmas (icpc): 5.4x
- Optimized code generated by a DSL compiler (PolyMage): tiling + fusion + scratchpads, etc. (**2.27**$\times$ over naive)
- Enhancements in PolyMage: + storage opt + pooled memory + multidim parallelism, etc. (**5.92**$\times$ over naive)

Naive vs Optimized Implementation



Multigrid-2D (Jacobi) (24 cores)

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- **Problem: Speeding up complex pipelines like multigrid cycles manually is hard and tedious**
- **Goal: Figure out complex and right set of optimizations automatically**

Related Work

Semi-automatic ones

- **S. Williams, D. Kalamkar et al. [SC 2012]**
  Communication aggregation: for dist-mem
  Wavefront schedule at node
  Fusion of Residual and Restrict
  Manual optimization and implementations
- **Ghysels and Vanroose [SIAM J. Scientific Computing 2015]**
  Pluto tiling for smoothing steps
  Manual optimization and implementation
  Code modifications for array access
- **P. Basu, M. Hall et al. [HiPC'13, IPDPS'15]**
  Wavefront schedule, fusion
  Semi-automatic (script-driven)
  No tiling transformations

Outline

Using PolyMage DSL to Optimize MG Cycles

- **PolyMage** [ASPLOS 2015]: DSL/Compiler for image processing pipelines
  - **DSL embedded in Python**
  - **Automatic Optimizing Code Generator**
    - Uses domain-specific cost models to apply complex combinations of **tiling** and **fusion** to optimize for **parallelism** and **locality**

PolyMage for Multigrid

- Express grid computations as functions
- Abstracts away computations from schedule and storage mapping
- Added new constructs for time-iterated stencils (smoothing)
- Use the **polyhedral framework** to transform, optimize, and parallelize

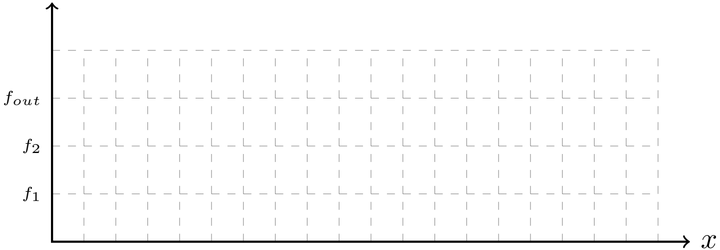
  Group functions, tile each group, generate storage mappings

V-cycle Algorithm in PolyMage

```
N = Parameter(Int, 'n')
V = Grid(Double, "V", [N+2, N+2])
F = Grid(Double, "F", [N+2, N+2])
...
def rec_v_cycle(v, f, l):
    # coarsest level
    if l == 0:
        smooth_p1[l] = smoother(v, f, l, n3)
        return smooth_p1[l][n3]
    # finer levels
    else:
        smooth_p1[l] = smoother(v, f, l, n1)
        r_h[l] = defect(smooth_p1[l][n1], f, l)
        r_2h[l] = restrict(r_h[l], l)
        e_2h[l] = rec_v_cycle(None, r_2h[l], l-1)
        e_h[l] = interpolate(e_2h[l], l)
        v_c[l] = correct(smooth_p1[l][n1], e_h[l], l)
        smooth_p2[l] = smoother(v_c[l], f, l, n2)
        return smooth_p2[l][n2]

def restrict(v, l):
    R = Restrict(([y, x], [extent[l], extent[l]]),
                 Double)
    R.defn = [ Stencil(v, (y, x),
                 [[1, 2, 1],
                  [2, 4, 2],
                  [1, 2, 1]], 1.0/16, factor=1//2) ]
    return R
```

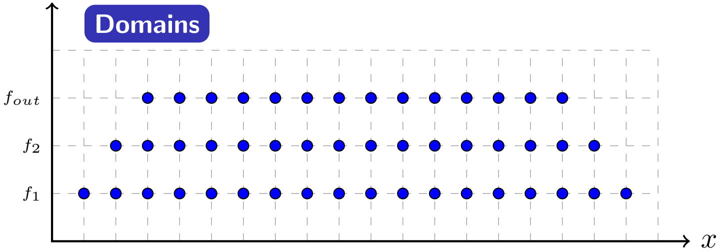
```
def smoother(v, f, l, n):
  ...
  W = TStencil(([y, x], [extent[l], extent[l]]),
               Double, T)
  W.defn = [ v(y, x) - weight *
    (Stencil(v, [y, x],
      [[ 0, -1,  0],
       [-1,  4, -1],
       [ 0, -1,  0]], 1.0/h[l]**2) - f(y, x)) ]
  ...
  return W

def interpolate(v, l):
    ...
    expr = [{}, {}]
    expr[0][0] = Stencil(v, (y, x), [1])
    expr[0][1] = Stencil(v, (y, x), [1, 1]) \
                 * 0.5
    expr[1][0] = Stencil(v, (y, x), [[1], [1]]) \
                 * 0.5
    expr[1][1] = Stencil(v, (y, x), [[1, 1], [1, 1]])\
                 * 0.25
    P = Interp(([y, x], [extent[l], extent[l]]),
               Double)
    P.defn = [ expr ]
    return P
```

Polyhedral Representation




```
x = Variable()
f_in = Grid(Double, [18])
f_1 = Function(([x], [Interval(0, 17)]), Double)
f_1.defn = [ f_in(x) + 1 ]
f_2 = Function(([x], [Interval(1, 16)]), Double)
f_2.defn = [ f_1(x-1) + f_1(x+1) ]
f_out = Function(([x], [Interval(2, 15)]), Double)
f_out.defn = [ f_2(x-1) . f_2(x+1) ]
```

Polyhedral Representation

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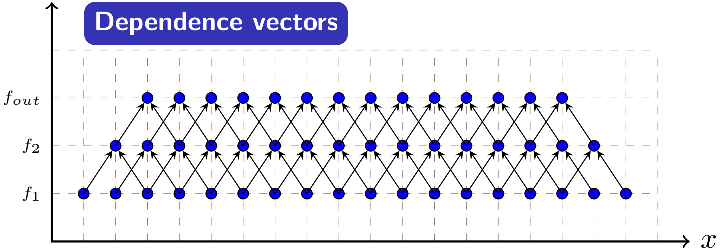
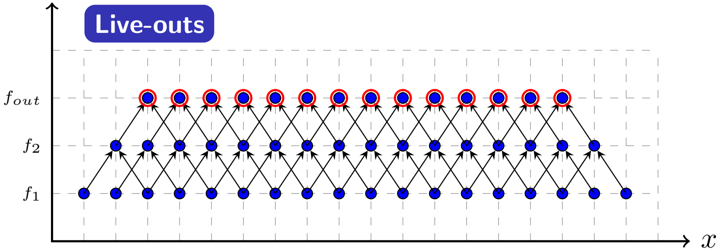
Polyhedral Representation



Function	Dependence Vectors
$f_{out}(x) = f_2(x-1) \cdot f_2(x+1)$	$(1,1),(1,-1)$
$f_2(x) = f_1(x-1) + f_1(x+1)$	$(1,1),(1,-1)$
$f_1(x) = f_{in}(x)$	

Polyhedral Representation



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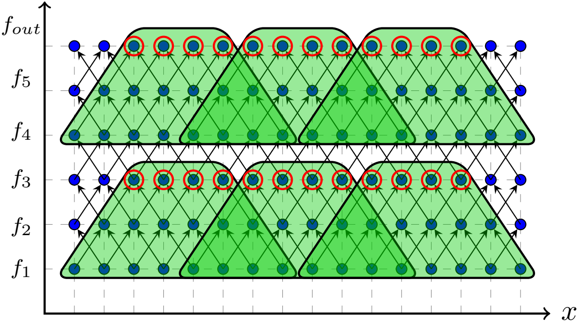
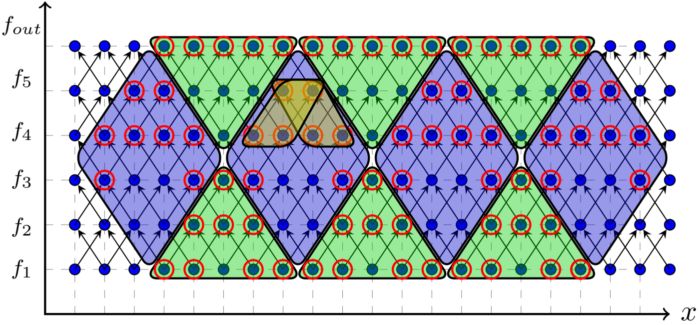
Tiling Smoothing Steps: Overlapped Tiling



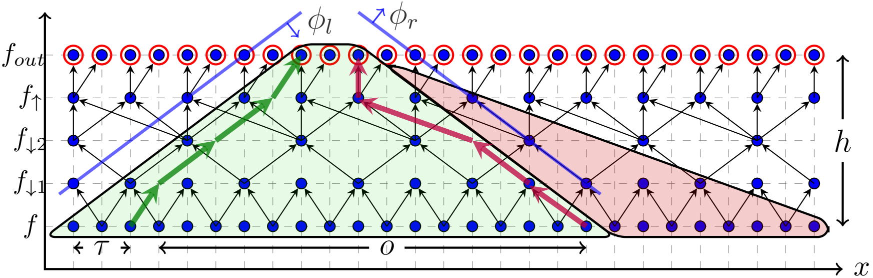
- Good for parallelism, locality, local buffers
- Redundant computation at boundaries

Tiling Smoothing Steps: Diamond Tiling



- Good for parallelism, locality, but not local buffers
- No redundant computation

Overlapped Tiling for Multiscale



Grouping Stages for Overlapped Tiling

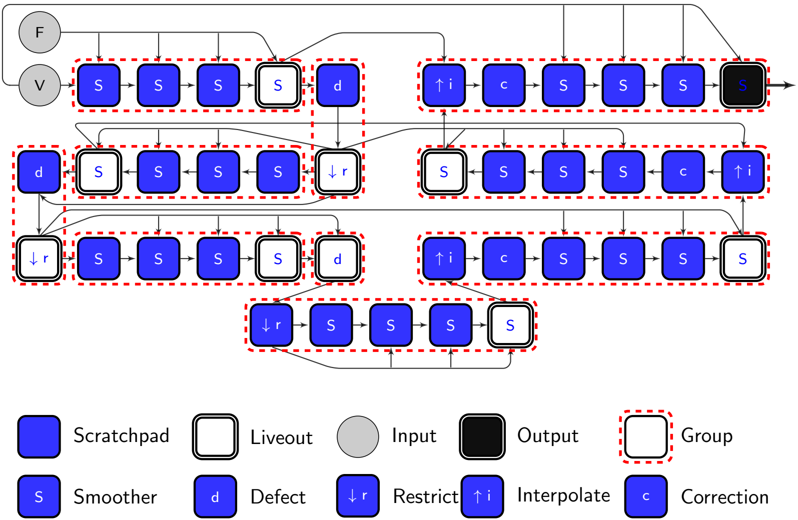
Grouping criteria

- Exponential number of valid groupings
- Redundant computation vs reuse (locality)
  Overlap, tile sizes, parameter estimates

Grouping heuristic

- Greedy iterative algorithm
- Only fuse stages that can be overlap
  tiled up to a maximum group size limit

Grouping



F
V
S
d
↓ r
↑ i
c
Scratchpad
Liveout
Input
Output
Group
Smoother
Defect
Restrict
Interpolate
Correction

Storage Optimizations

- **Storage for Functions**
  - Reuse of buffers across groups and witihn groups
  - Precise liveness information is available

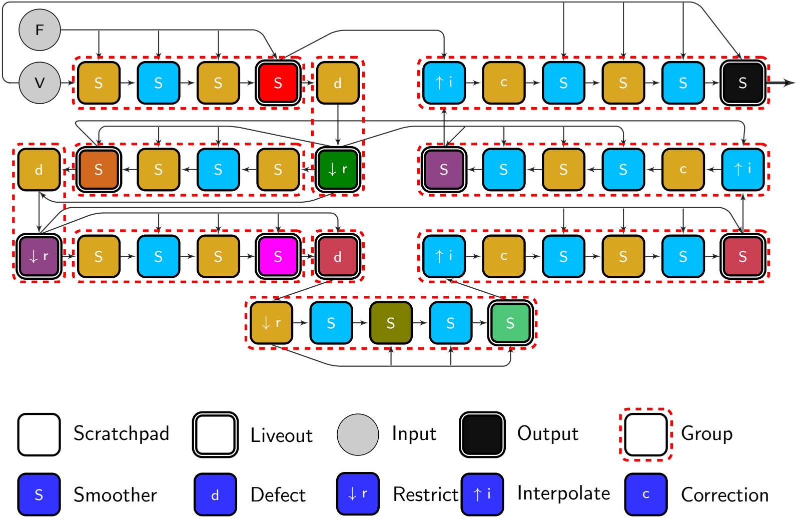
Intra-Group Storage Reuse

- **Not just about byte count**
  - Accommodate larger tile sizes
  - Maximum performance gains for a configuration
- **Approach**
  - Simple greedy algorithm to colour the nodes
  - Requires schedule information

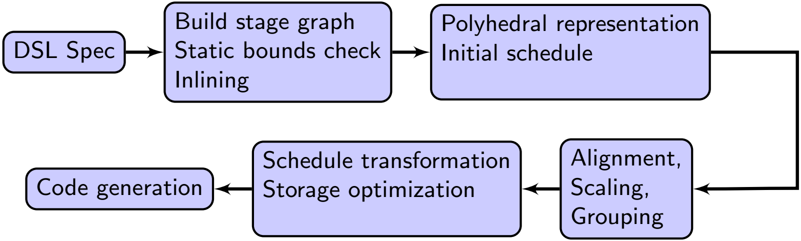
Inter-Group Storage Reuse

- **Larger gains in memory used**
  - Significant reduction in memory consumption
  - Less page activity
  - Higher chances of fitting in LLC
- **Approach**
  - Classification based on parametric bounds
  - Alloc/free at group granularity
- Pooled allocation and early freeing: across multiple calls and within pipeline call

Storage Allocation for Grouping



PolyMage Compiler Flow



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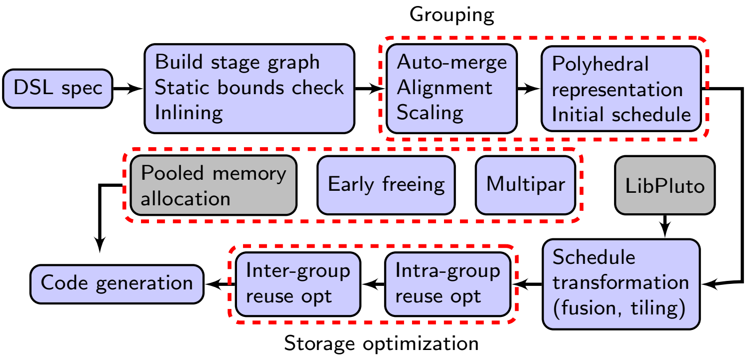


Availability

- Available as part of PolyMage repository
  https://bitbucket.org/udayb/polymage.git

  Multigrid benchmarks
  sandbox/apps/python/multigrid/

Outline

Benchmarks

- **Multigrid applications solving Poisson's equation**

$$\nabla^2 u = f.$$

- **Configurations**
  - V-cycle and W-cycle
  - 10-0-0 and 4-4-4
  - Four levels of discretization
- **NAS-MG from NAS-PB 3.2**

Benchmarks

Table: Problem size configurations: the same problem sizes were used for V-cycle and W-cycle and for 4-4-4 and 10-0-0

Benchmark	Grid size, cycle #iters	
	Class B	Class C
2D	8192^2 (10)	16384^2 (10)
3D	256^3 (25)	512^3 (10)
NAS-MG	256^3 (20)	512^3 (20)

Experimental Setup

Table: Architecture details

	2-socket Intel Xeon E5-2690 v3
Clock	2.60 GHz
Cores / socket	12
Total cores	24
Hyperthreading	disabled
L1 cache / core	64 KB
L2 cache / core	512 KB
L3 cache / socket	30,720 KB
Memory	96 GB DDR4 ECC 2133 MHz
Compiler	Intel C/C++ and Fortran compiler (icc/icpc and ifort) 16.0.0
Compiler flags	-O3 -xhost -openmp -ipo
Linux kernel	3.10.0 (64-bit) (Cent OS 7.1)

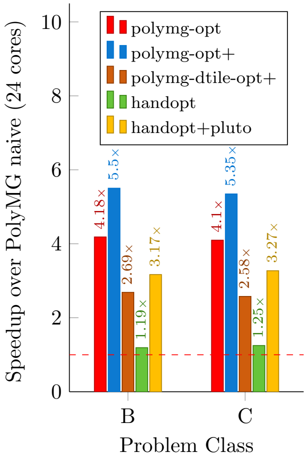
Lines of Code

Benchmark	Stages (= # of DAG nodes)	Lines of code: PolyMage DSL (Python)	Lines of code: HandOpt (C)	Lines of code: HandOpt + Pluto (C)	Lines of generated code: *polymage-opt* (C/C++)	Lines of generated code: *polymage-opt+* (C/C++)
V-2D-4-4-4	40	160	140	150	2324	2496
V-2D-10-0-0	42				2155	2059
W-2D-4-4-4	100	165	145	155	6156	6768
W-2D-10-0-0	98				4306	4711
V-3D-4-4-4	40	220	185	200	4889	4457
V-3D-10-0-0	42				4593	4179
W-3D-4-4-4	100	225	190	205	12184	11535
W-3D-10-0-0	98				9237	7897
NAS-MG	34	180	500	-	2010	2013

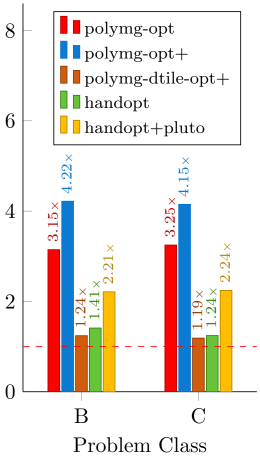
Comparison with Hand Opt and Pluto

- **Ghysels and Vanroose [SIAM J. Sci. Comp. 2015]**
  - Manual storage reuse optimization
  - Multidimensional parallelism
  - **Pluto**
    - Diamond tiling for concurrent startup
    - Tuned over 25 tile size configurations

2D Benchmarks: V-cycle

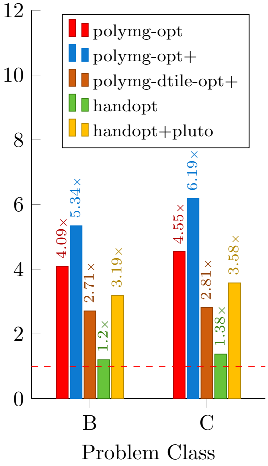


(a) 2D-V-10-0-0

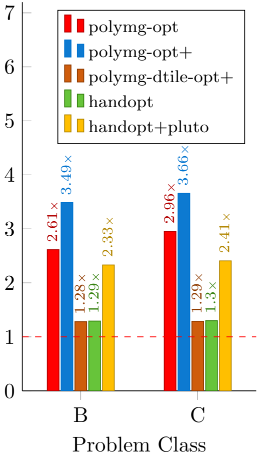


(b) 2D-V-4-4-4

2D Benchmarks: W-cycle

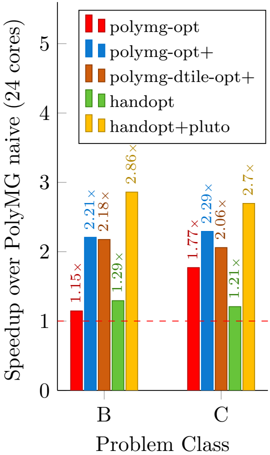


(c) 2D-W-10-0-0

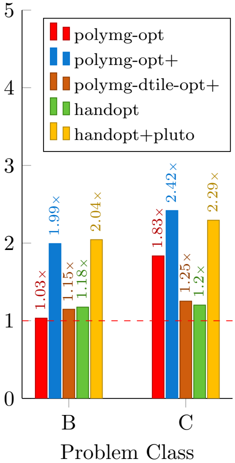


(d) 2D-W-4-4-4

3D Benchmarks: V-cycle

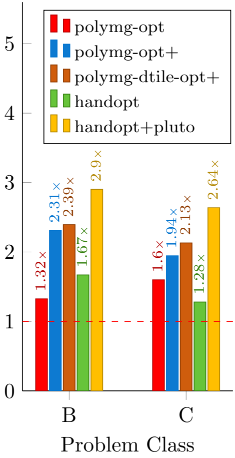


(e) 3D-V-10-0-0

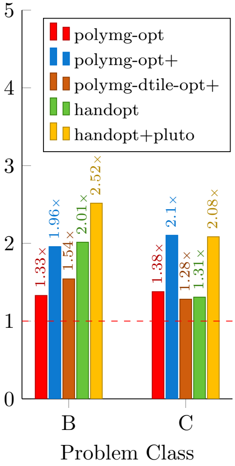


(f) 3D-V-4-4-4

3D Benchmarks: W-cycle

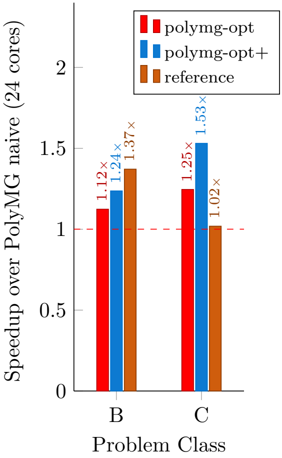


(g) 3D-W-10-0-0



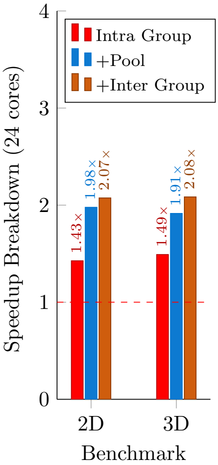
(h) 3D-W-4-4-4

NAS-MG



polymg-opt
polymg-opt+
reference
Speedup over PolyMG naive (24 cores)
0
0.5
1
1.5
2
1.12×
1.24×
1.37×
1.25×
1.53×
1.02×
B
C
Problem Class

Storage Optimization Gains



V-cycle for 10-0-0

Summary of Improvements

- **1.31**$\times$ Mean speedup of **Opt+** over **Opt**
  - **1.30**$\times$: 2D
  - **1.33**$\times$: 3D
- **3.21**$\times$ Mean speedup of **Opt+** over **Naive**
  - **4.74**$\times$: 2D
  - **2.18**$\times$: 3D
- **1.23**$\times$ Mean speedup of **Opt+** over **HandOpt+Pluto**
- **NAS-MG 17%** better over **Opt+**

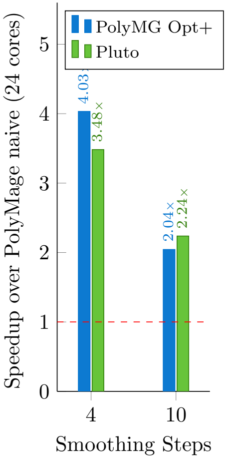
Conclusions

- **Conclusions**
  - Significant performance improvement (automatic) through DSL approach
  - Overlapped tiling - very effective for 2D GMG
  - Diamond tiling better than Overlapped tiling for most of the 3D benchmarks
  - Storage allocation and optimization - important for performance
- **Future Directions**
  - Distributed memory

Thank You

Acknowledgments

Tiling Smoothing Steps



3D stencil for class C

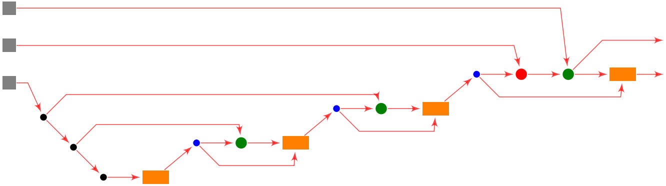
Sample Output

```
void pipeline_Vcycle(int N, double * F,
                     double * V, double *& W)
{
  /* Live out allocation */
  /* users : ['T9_pre_L3'] */
  double * _arr_10_2;
  _arr_10_2 = (double *) (pool_allocate(sizeof(double) *
                          (2+N)*(2+N)));
#pragma omp parallel for schedule(static) collapse(2)
  for (int Ti = -1; Ti <= N/32; Ti+=1) {
    for (int Tj = -1; Tj <= N/512; Tj+=1) {
      /* Scratchpads */
      /* users : ['T8_pre_L3', 'T6_pre_L3', 'T4_pre_L3',
                  'T2_pre_L3', 'T0_pre_L3'] */
      double _buf_2_0[(50 * 530)];
      /* users : ['T7_pre_L3', 'T5_pre_L3', 'T3_pre_L3',
                  'T1_pre_L3'] */
      double _buf_2_1[(50 * 530)];

      int ubi = min(N, 32*Ti + 49);
      int lbi = max(1, 32*Ti);
      for (int i = lbi; i <= ubi; i+=1) {
        int ubj = min(N, 512*Tj + 529);
        int lbj = max(1, 512*Tj);
#pragma ivdep
        for (int j = lbj; (j <= ubj); j+=1) {
          _buf_2_0[(-32*Ti+i)*530 + -512*Tj+j] = ...;
        }}

      int ubi = min(N, 32*Ti + 48);
      int lbi = max(1, 32*Ti);
      for (int i = lbi; i <= ubi; i+=1) {
        int ubj = min(N, 512*Tj + 528);
        int lbj = max(1, 512*Tj);
#pragma ivdep
        for (int j = lbj; (j <= ubj); j+=1) {
          _buf_2_1[(-32*Ti+i)*530 + -512*Tj+j] = ...;
        }}
      ...
  }}
  ...
  pool_deallocate(_arr_10_2);
  ...
}
```

NAS-MG V-Cycle



Smoother

Defect/Residual

Correction

Restrict/Reciprocate

Interpolate/Prolongation