Whole Program Generation for Complex Fluid Flow Solvers

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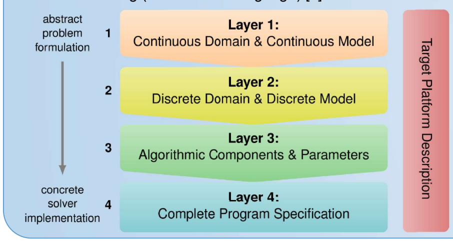
Project ExaStencils

Generation of efficient, robust and exa-scalable geometric multigrid solvers [1] from abstract inputs in our multi-layered DSL ExaSlang (ExaStencils Language) [2]



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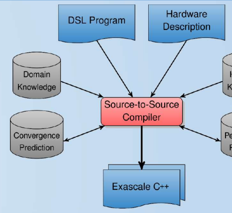


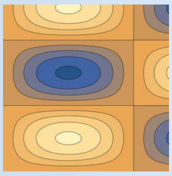
- Modular code generation framework based on fine-grained transformations
- Automatic parallelization via MPI/OMP [3] and/or CUDA
- Automatic low-level optimizations (polyhedral loop transformations, vectorization, CSE, APC, etc.) [4]
- Interfacing with performance prediction models

Problem Specification

We consider the following problems:

(1) a steady-state Stokes flow with the (known) solution:

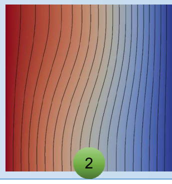
$$\begin{aligned} u &= -4\cos(4z) \\ v &= 8\cos(8x) \\ w &= -2\cos(2y) \\ p &= \sin(4x)\sin(8y)\sin(2z) \end{aligned}$$

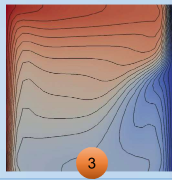


$$\begin{aligned} -\Delta u + \frac{\partial u}{\partial x} &= f_u \\ -\Delta v + \frac{\partial v}{\partial y} &= f_v \\ -\Delta w + \frac{\partial w}{\partial z} &= f_z \\ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} &= f_p \end{aligned}$$

(2) a non-isothermal/ non-Newtonian fluid flow following the specifications in [6]
we choose a natural convection test-case (a flow is induced by heating one wall and cooling another)

(3) a non-isothermal/ Newtonian fluid flow, equivalent to (2) disregarding the non-Newtonian properties





Discretization

```
Stencil Au@all { /* stencil coefficients are not stored */
  [ 1,  0,  0] => integrateOverXStaggeredEastFace   ( -1.0 )
                  / vf_cellWidth_x@[1, 0, 0]
  [-1,  0,  0] => integrateOverXStaggeredWestFace   ( -1.0 )
                  / vf_cellWidth_x@[0, 0, 0]
  [ 0,  1,  0] => integrateOverXStaggeredNorthFace  ( -1.0 )
                  / vf_stagCVWidth_y@[0, 1, 0]
  [ 0, -1,  0] => integrateOverXStaggeredSouthFace  ( -1.0 )
                  / vf_stagCVWidth_y@[0, 0, 0]
  [ 0,  0,  1] => integrateOverXStaggeredTopFace    ( -1.0 )
                  / vf_stagCVWidth_z@[0, 0, 1]
  [ 0,  0, -1] => integrateOverXStaggeredWestBottom ( -1.0 )
                  / vf_stagCVWidth_z@[0, 0, 0]

  [ 0,  0,  0] => /* negative sum of other entries */
}
```

(1)

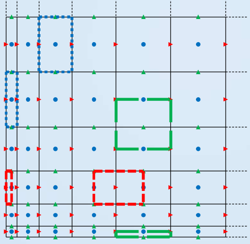
```
Stencil Cu@all { /* dx from xStag to Cell */
  [ 0,  0,  0] => -vf_cellWidth_y * vf_cellWidth_z
  [ 1,  0,  0] =>  vf_cellWidth_y * vf_cellWidth_z
}
```

(1) (2) (3)

To obtain the discretized version

$$\begin{bmatrix} A_u & 0 & 0 & B_u \\ 0 & A_v & 0 & B_v \\ 0 & 0 & A_w & B_w \\ C_u & C_v & C_w & 0 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \\ p \end{bmatrix} = \begin{bmatrix} rhs_u \\ rhs_v \\ rhs_w \\ rhs_p \end{bmatrix}$$

We apply a finite volume discretization on non-uniform, axis-aligned, staggered grids

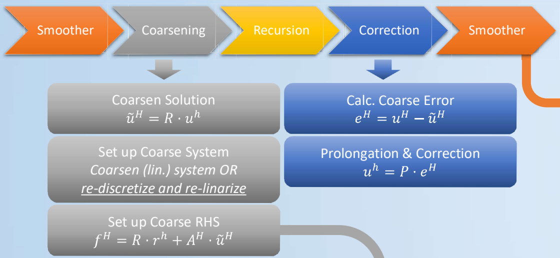


```
Function AssembleAu@all { /* stencil coefficients are stored in a dedicated field */
  loop over Au {
    Val flow_e = integrateOverXStaggeredEastFace ( u * rho )
    Val flow_w = integrateOverXStaggeredWestFace ( u * rho )
    Val diff_e = integrateOverXStaggeredEastFace ( vis ) / vf_cellWidth_x@[ 0,  0,  0]
    Val diff_w = integrateOverXStaggeredWestFace ( vis ) / vf_cellWidth_x@[-1,  0,  0]

    Au:[ 1,  0,  0] = -calc_diflow ( flow_e, diff_e ) + max ( 0.0, -flow_e )
    Au:[-1,  0,  0] = -calc_diflow ( flow_w, diff_w ) + max ( 0.0,  flow_w )

    Val flow_n = integrateOverXStaggeredNorthFace ( v * rho )
    Val flow_s = integrateOverXStaggeredSouthFace ( v * rho )
    Val diff_n = ( integrateOverXStaggeredNorthFace (
                   evalAtXStaggeredNorthFace ( vis, "harmonicMean" ) )
                   / vf_stagCVWidth_y@[ 0,  1,  0] )
    Val diff_s = ( integrateOverXStaggeredSouthFace (
                   evalAtXStaggeredSouthFace ( vis, "harmonicMean" ) )
                   / vf_stagCVWidth_y@[ 0,  0,  0] )

    Au:[ 0,  1,  0] = -calc_diflow ( flow_n, diff_n ) + max ( 0.0, -flow_n )
    Au:[ 0, -1,  0] = -calc_diflow ( flow_s, diff_s ) + max ( 0.0,  flow_s )

    /* other components */
  }}
```

(2) (3)

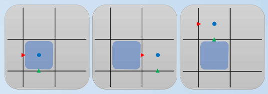
Solver

- A standard geometric multigrid is sufficient for (1)
- A full approximation scheme (FAS) multigrid is required for (2) and (3)
- In all cases, (colored) Vanka smoothers can be employed




```
uApprox@coarser = RestrictionFaceX * u
/* other components */

res_u = rhs_u - Au * u - Bu * p
/* other components */

rhs_u@coarser = ( RestrictionFaceXInteg * res_u
                + Au@coarser * uApprox@coarser
                + Bu@coarser * pApprox@coarser )
/* other components */
```

(2) (3)




```
color with {
  0 == ( i0 + i1 + i2 ) % 2,
  1 == ( i0 + i1 + i2 ) % 2,

  loop over p {
    solve locally relax 0.8 {
      u@[0, 0, 0] => Au@[0, 0, 0] * u@[0, 0, 0] + Bu@[0, 0, 0] * p@[0, 0, 0] == rhs_u@[0, 0, 0]
      u@[1, 0, 0] => Au@[1, 0, 0] * u@[1, 0, 0] + Bu@[1, 0, 0] * p@[1, 0, 0] == rhs_u@[1, 0, 0]

      v@[0, 0, 0] => Av@[0, 0, 0] * v@[0, 0, 0] + Bv@[0, 0, 0] * p@[0, 0, 0] == rhs_v@[0, 0, 0]
      v@[0, 1, 0] => Av@[0, 1, 0] * v@[0, 1, 0] + Bv@[0, 1, 0] * p@[0, 1, 0] == rhs_v@[0, 1, 0]

      /* similar for w */

      p => Cu * u + Cv * v + Cw * w == rhs_p
}}}
```

(1) (2) (3)

Mapping to code

- Preprocessing – apply coloring via duplication
- Set up the (local) LSE
  - Preprocessing – unfold nested expressions
  - Identify unknowns and reorder equations
  - Apply simplifications
- Check for suitability to apply **Schur complement** to accelerate local solve
- Incorporate (inner) boundaries
- Generate code to write back the results

$$\begin{bmatrix} A_{11} & 0 & 0 & B_1 \\ 0 & A_{22} & 0 & B_2 \\ 0 & 0 & A_{33} & B_3 \\ C_1 & C_2 & C_3 & D \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ V \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ G \end{bmatrix}$$

$$S = D - (C_1 A_{11}^{-1} B_1 + C_2 A_{22}^{-1} B_2 + C_3 A_{33}^{-1} B_3)$$

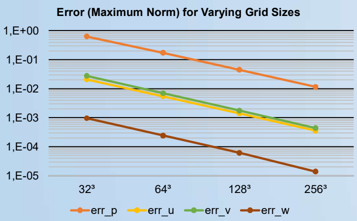
$$\tilde{G} = G - (C_1 A_{11}^{-1} F_1 + C_2 A_{22}^{-1} F_2 + C_3 A_{33}^{-1} F_3)$$

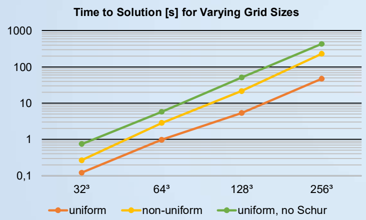
$$V = S^{-1} \tilde{G}$$

$$\begin{aligned} U_1 &= A_{11}^{-1}(F_1 - B_1 V) \\ U_2 &= A_{22}^{-1}(F_2 - B_2 V) \\ U_3 &= A_{33}^{-1}(F_3 - B_3 V) \end{aligned}$$

Results

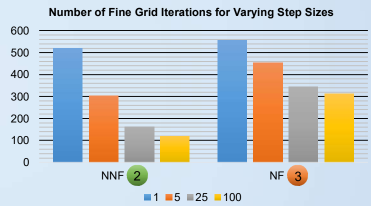
Solves (1) for the steady state using v(4,4)-cycles and a RB Vanka smoother

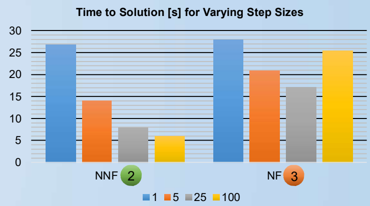




Solves (2) (3) for the first 100s on 32³ cells using

- FMG for the first time step
- RB Vanka as smoother for u,v,w,p
- RB GS as smoother for the temperature
- truncated v((2,5),(2,5))-cycles





Evaluation platform: single Intel Xeon E5-2623 v3 socket with 4 cores @3.0 GHz; no optimizations applied; automatic (OpenMP) parallelization using 4 threads

References

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[2] Schmitt C, Kuckuk S, Hannig F, Köstler H, Teich J. *ExaSlang: A domain-specific language for highly scalable multigrid solvers*. Proc. of the Fourth International Workshop on Domain-Specific Languages and High-Level Frameworks for High Performance Computing (WOLFHPC), IEEE Computer Society, 2014; 42–51.
[3] Kuckuk S, Köstler H. *Automatic Generation of Massively Parallel Codes from ExaSlang*. Computation, 4(3):Article 27, 2016. Special Issue on High Performance Computing (HPC) Software Design.
[4] Kronawitter S, Lengauer C. *Optimizations applied by the ExaStencils code generator*. Technical Report MIP-1502, Faculty of Informatics and Mathematics, University of Passau 2015.
[5] Schmitt C, Kuckuk S, Hannig F, Teich J, Köstler H, Rüde U, and Lengauer C. *Systems of Partial Differential Equations in ExaSlang*. Software for Exascale Computing – SPPEXA 2013-2015, volume 113 of Lecture Notes in Computational Science and Engineering, Springer, 2016; 47–67
[6] Kuckuk S, Haase G, Vasco DA. *Towards generating efficient flow solvers with the ExaStencils Approach*. Concurrency and Computation: Practice and Experience, 2017. Special Issue on Advanced Stencil-Code Engineering; early view.