

Elmer/Ice User meeting Nov. 2023

Thomas Zwinger, CSC – IT Center for Science Ltd.



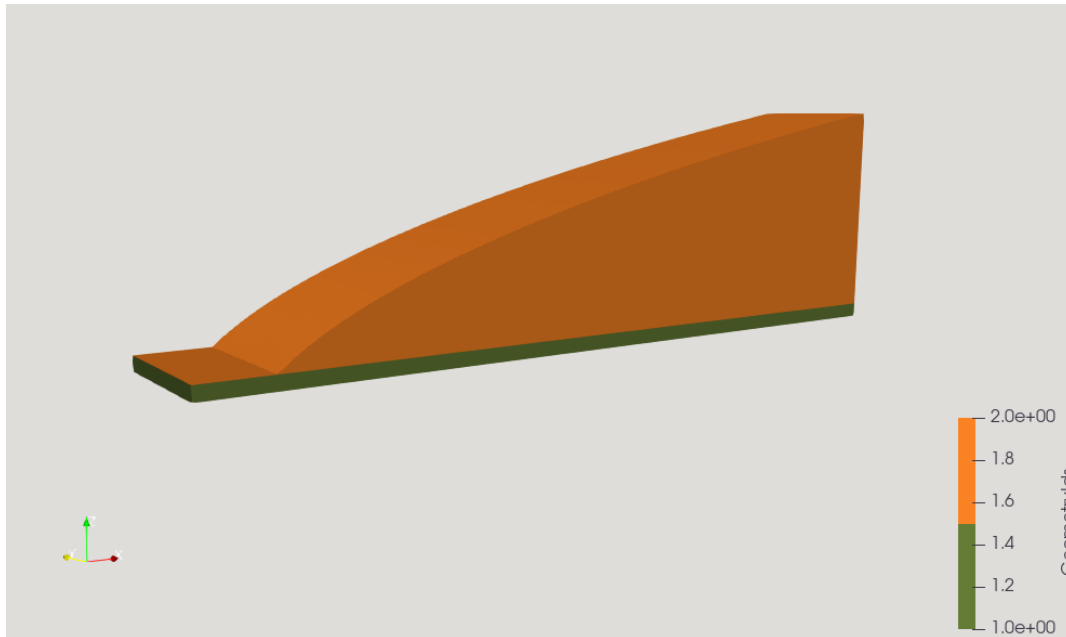
CSC – Suomalainen tutkimuksen, koulutuksen, kulttuurin ja julkishallinnon ICT-osaamiskeskus

Changes in internal extrusion

Thomas Zwinger

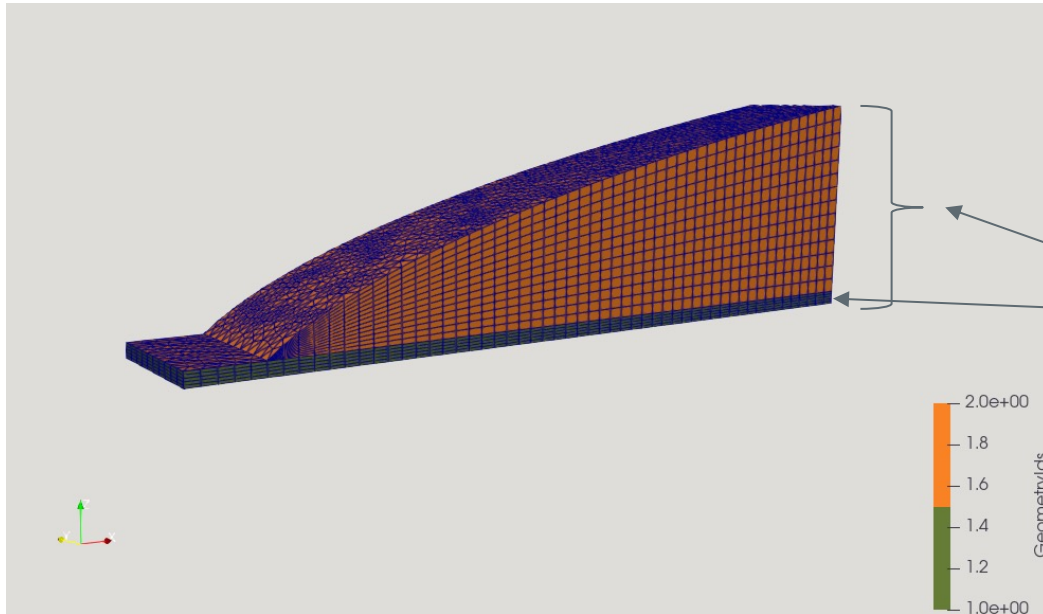


Changes in internal extrusion



- Possibility to include midlayer
- For instance, if one wants to add bedrock underneath ice-sheet/glacier
- Starting from 2D footprint
- Declaration in Simulation section

Changes in internal extrusion



```
extrusion_only.sif - emacs
File Edit Options Buffers Tools Help
!----- SIMULATION -----!
!----- SIMULATION -----!
Simulation
Coordinate System = Cartesian 3D
Simulation Type = transient

Timestepping Method = "bdf"
BDF Order = 1

Timestep Intervals(1) = #Iter

Timestep Sizes(1) = #dtIni

Steady State Max Iterations = 1
Steady State Min Iterations = 1

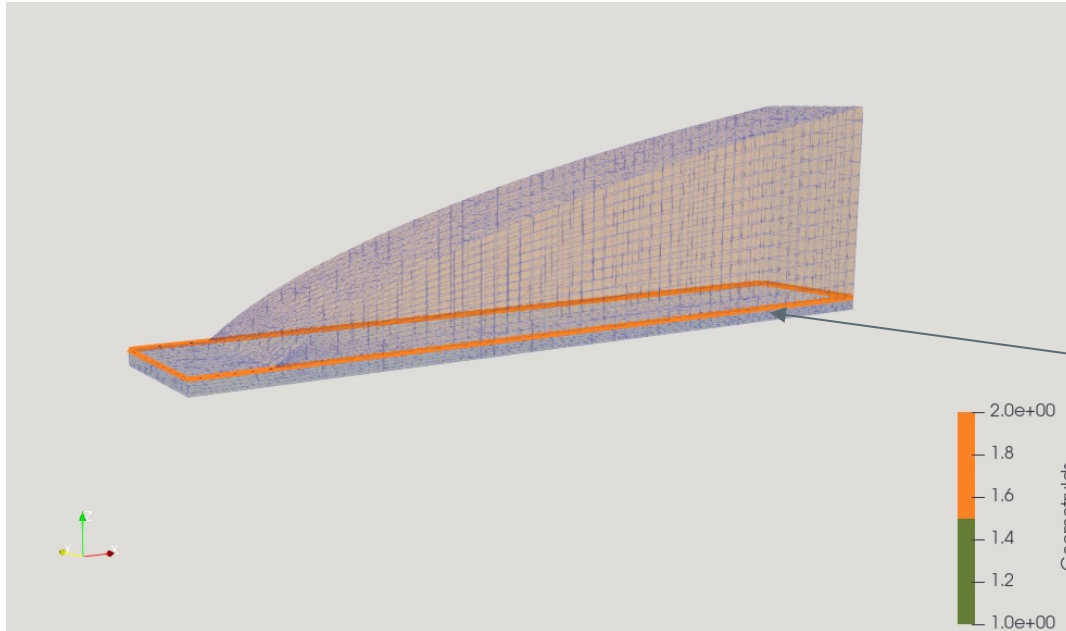
Extruded Mesh Levels = Integer 20
Extruded BC Layers(1) = Integer 5
Preserve Baseline = Logical True
Extruded Baseline Layer = Integer 2

Post File = "$namerun$.vtu"
Output File = "$namerun$.result"
!Output Intervals(1) = 30
Output Intervals(1) = #OutPut
max output level = 3
End

!----- BODIES -----!
!----- BODIES -----!

-:--- extrusion_only.sif 23% L124 (Sif)
```

Changes in internal extrusion



```
extrusion_only.sif - emacs
File Edit Options Buffers Tools Help
!----- SIMULATION -----!
!----- SIMULATION -----!
Simulation
Coordinate System = Cartesian 3D
Simulation Type = transient

Timestepping Method = "bdf"
BDF Order = 1

Timestep Intervals(1) = #Iter

Timestep Sizes(1) = #dtIni

Steady State Max Iterations = 1
Steady State Min Iterations = 1

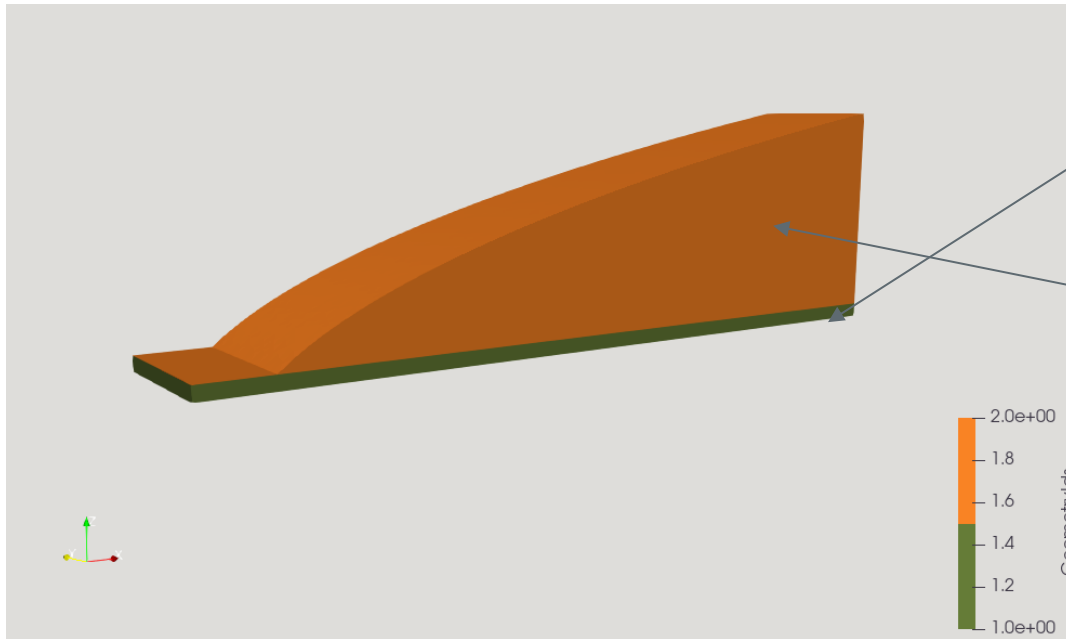
Extruded Mesh Levels = Integer 20
Extruded BC Layers(1) = Integer 5
Preserve Baseline = Logical True
Extruded Baseline Layer = Integer 2

Post File = "$namerun$.vtu"
Output File = "$namerun$.result"
!Output Intervals(1) = 30
Output Intervals(1) = #OutPut
max output level = 3
End

!----- BODIES -----!
!----- BODIES -----!

-:--- extrusion_only.sif 23% L124 (Sif)
```

Changes in internal extrusion



```

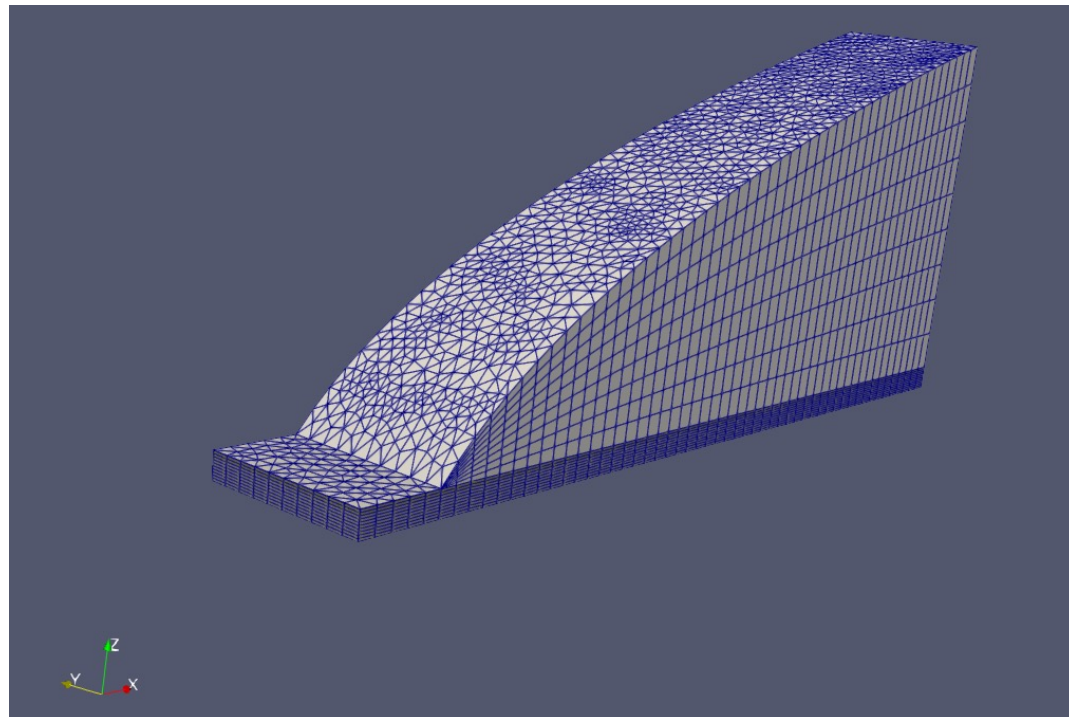
extrusion_only.sif - emacs
File Edit Options Buffers Tools Help
!-----
!----- BODIES -----
!-----
! This body is located at the ice/bed interface and will be used to solve
! the sheet equation

Body 1
  Name= "bedrock"
  Equation = 2
  Material = 2
  Initial Condition = 1
End
Body 2
  Name= "Ice"
  Equation = 1
  Material = 1
  Initial Condition = 1
End
Body 3
  Name= "sheet"
  Equation = 3
  Material = 1
  Body Force = 1
  Initial Condition = 1
End

!-----
!----- INITIAL CONDITIONS -----
!-----

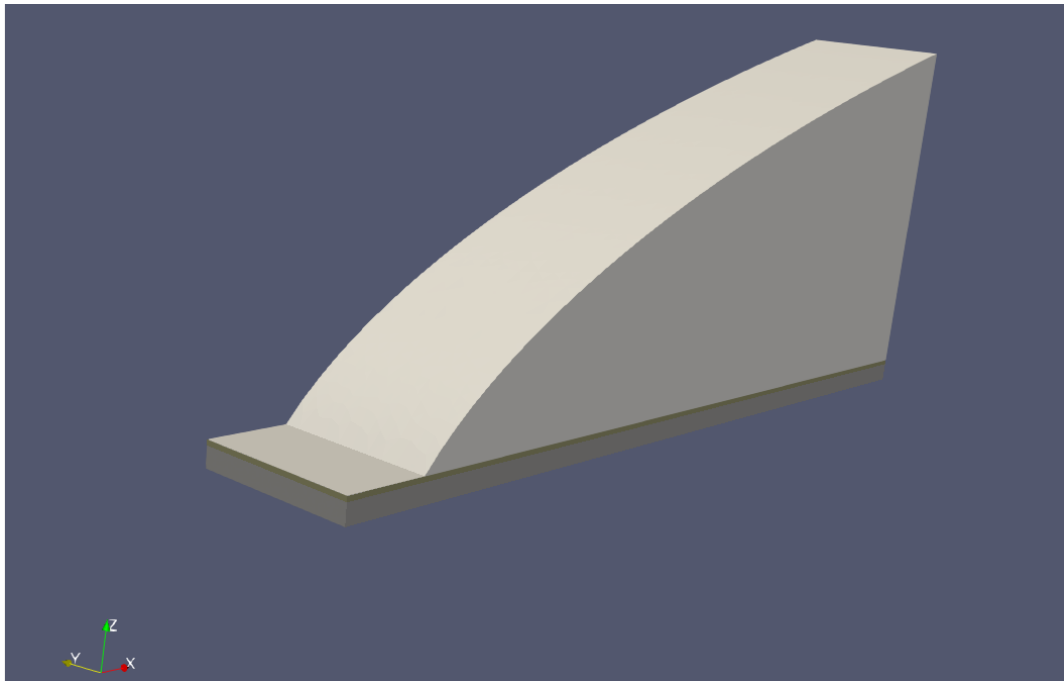
!! for the sheet
-:--- extrusion_only.sif 29% L156 (Sif)
  
```


Changes in internal extrusion



- Even more layers
- Here with 3 layers (ice + sediment + bedrock)

Changes in internal extrusion



```

extrusion3bdy_only.sif - emacs
File Edit Options Buffers Tools Help
!----- SIMULATION -----!
Simulation
Coordinate System = Cartesian 3D
Simulation Type = transient

Timestepping Method = "bdf"
BDF Order = 1

Timestep Intervals(1) = #Iter

Timestep Sizes(1) = #dtIni

Steady State Max Iterations = 1
Steady State Min Iterations = 1

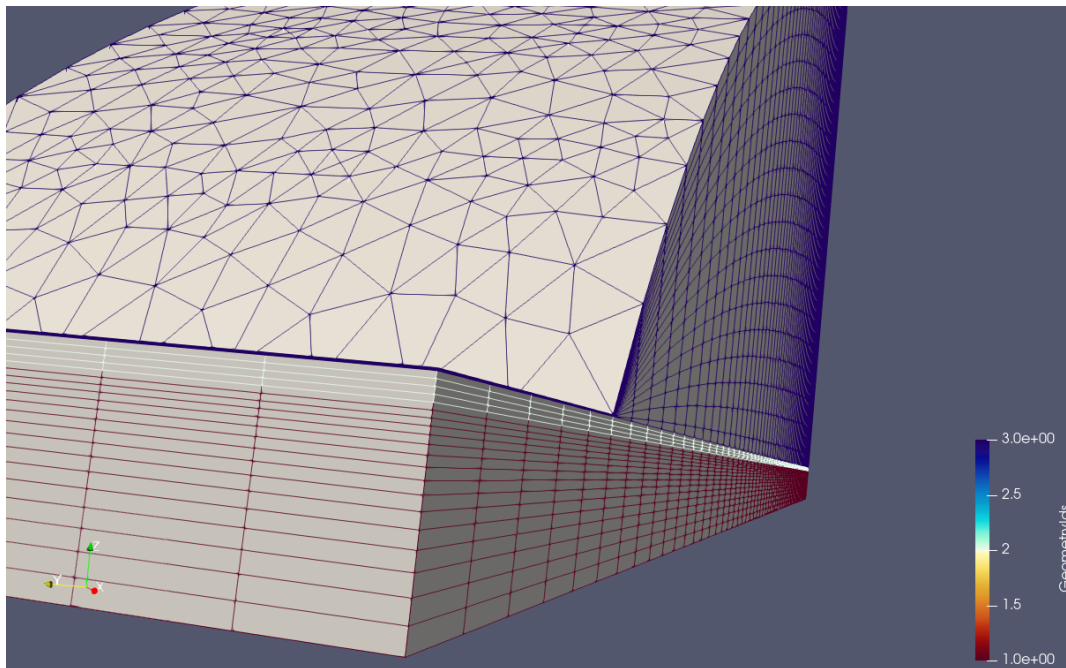
Extruded Mesh Levels = Integer 20
Extruded BC Layers(2) = Integer 8 10
Preserve Baseline = Logical True
Extruded Baseline Layer = Integer 3
Extruded Mesh Density = Variable Coordinate 1

Post File = "$namerun$.vtu"
Output File = "$namerun$.result"
!Output Intervals(1) = 30
Output Intervals(1) = #OutPut
max output level = 3

End
!-----
-:--- extrusion3bdy_only.sif 22% L135 (Sif)

```


Changes in internal extrusion



With mesh distribution

```
extrusion3bdy_only.sif - emacs
File Edit Options Buffers Tools Help
!-----
!----- SIMULATION -----
!-----
Simulation
Coordinate System = Cartesian 3D
Simulation Type = transient

Timestepping Method = "bdf"
BDF Order = 1

Timestep Intervals(1) = #Iter

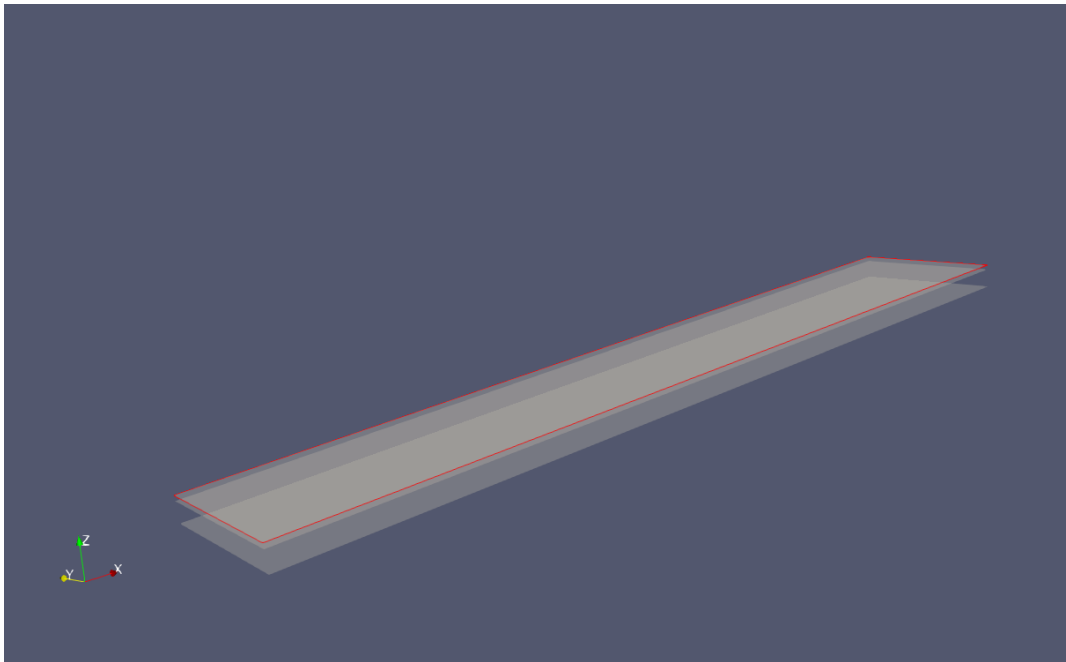
Timestep Sizes(1) = #dtIni

Steady State Max Iterations = 1
Steady State Min Iterations = 1

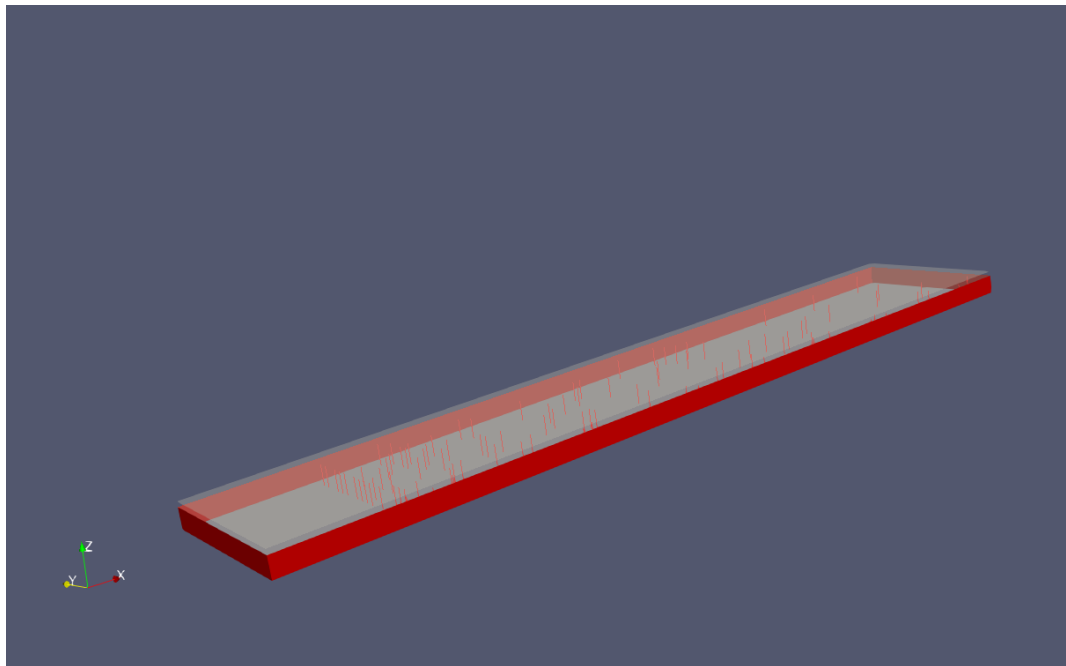
Extruded Mesh Levels = Integer 40
Extruded BC Layers(2) = Integer 16 20
Preserve Baseline = Logical True
Extruded Baseline Layer = Integer 3
Extruded Mesh Density = Variable Coordinate 1
  Real
    0.0 2.0
    0.39999 0.5
    0.49999 0.5
    0.5 1.0
    1.0 1.0
  End
Post File = "$namerun$.vtu"
Output File = "$namerun$.result"
!Output Intervals(1) = 30
Output Intervals(1) = #OutPut
-:--- extrusion3bdy_only.sif 22% L138 (Sif)
Wrote /home/zwinger/Work/Glaciology/GlaDS/GlaDS_comp/extrusion3bdy_only.sif
```

Changes in internal extrusion

- Baseline (BC 1-4): 3 sides and moulins as points (not visible)

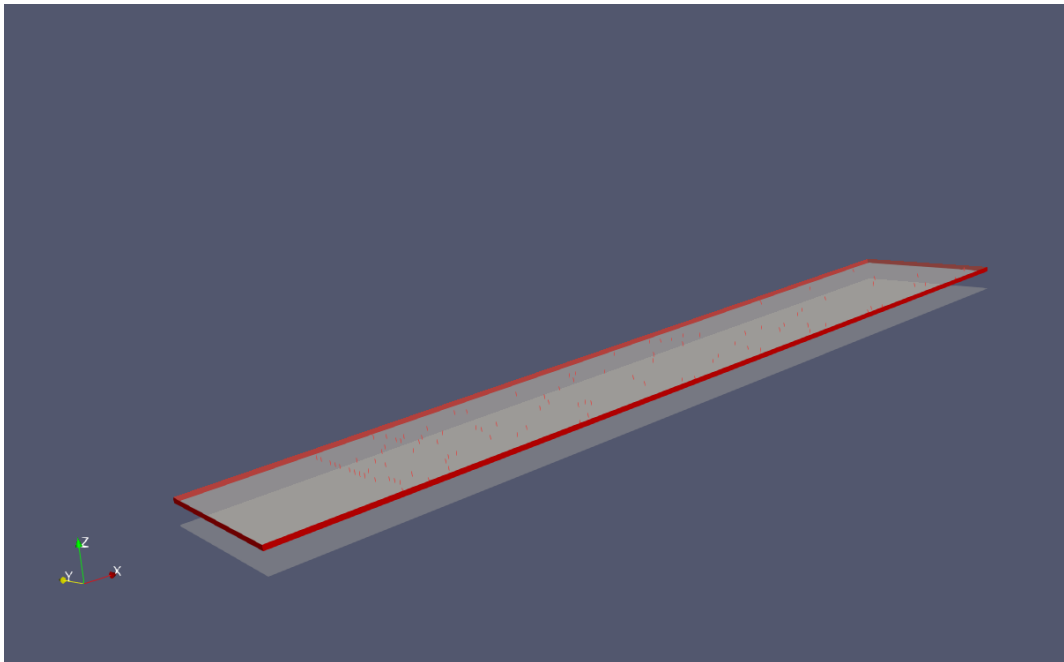


Changes in internal extrusion



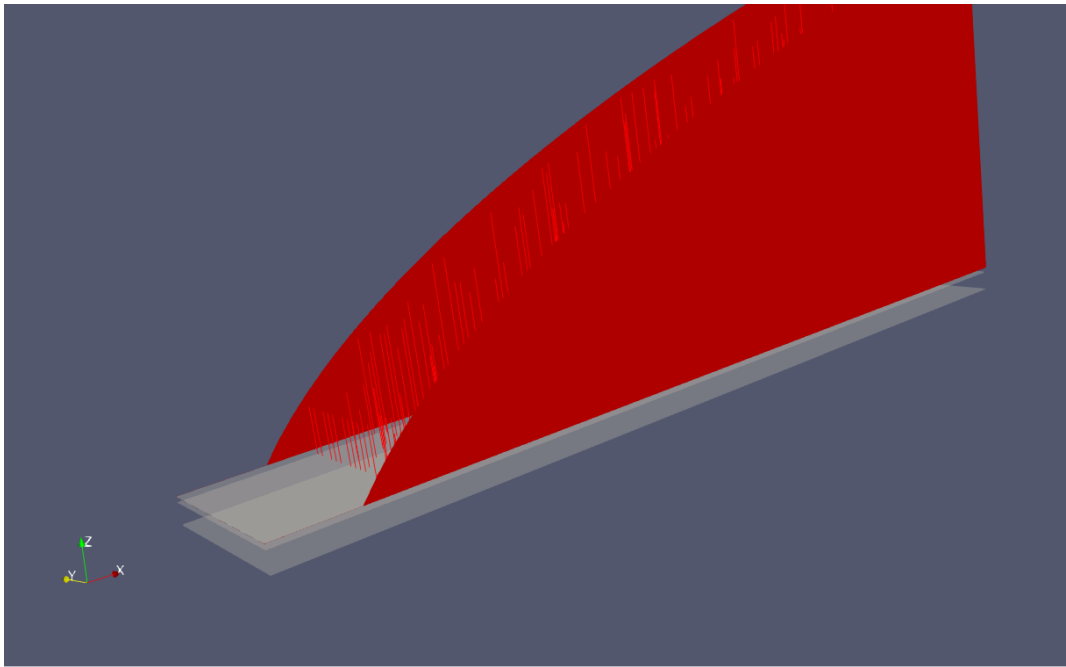
- Baseline (BC 1-4): 3 side-lines and moulins as points (not visible)
- Lowest part of extrusion (bedrock, BC 5-8): 3 sides + lines of moulins

Changes in internal extrusion



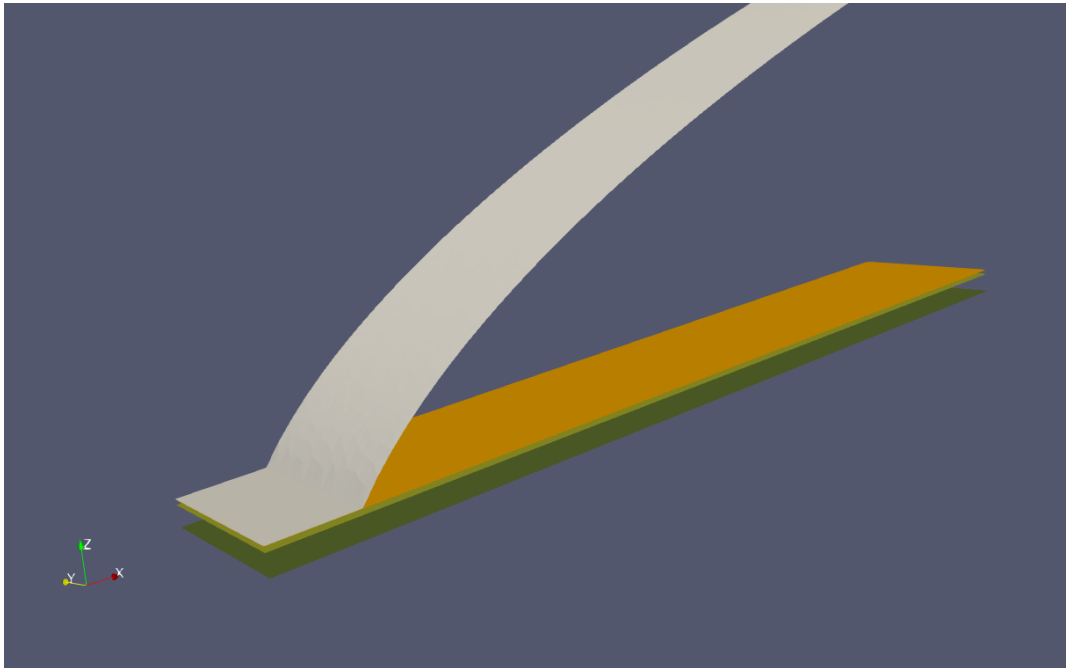
- Baseline (BC 1-4): 3 side-lines and moulins as points (not visible)
- Lowest part of extrusion (bedrock, BC 5-8): 3 sides + lines of moulins
- Middle part of extrusion (sediment, BC 9-12): 3 sides + lines of moulins

Changes in internal extrusion



- Baseline (BC 1-4): 3 side-lines and moulins as points (not visible)
- Lowest part of extrusion (bedrock, BC 5-8): 3 sides + lines of moulins
- Middle part of extrusion (sediment, BC 9-12): 3 sides + lines of moulins
- Upper part of extrusion (ice, BC 13-16): 3 sides + lines of moulins

Changes in internal extrusion



- Baseline (BC 1-4): 3 side-lines and moulins as points (not visible)
- Lowest part of extrusion (bedrock, BC 5-8): 3 sides + lines of moulins
- Middle part of extrusion (sediment, BC 9-12): 3 sides + lines of moulins
- Upper part of extrusion (ice, BC 13-16): 3 sides + lines of moulins
- Horizontal surfaces (BC 17-20): bottom until free surface

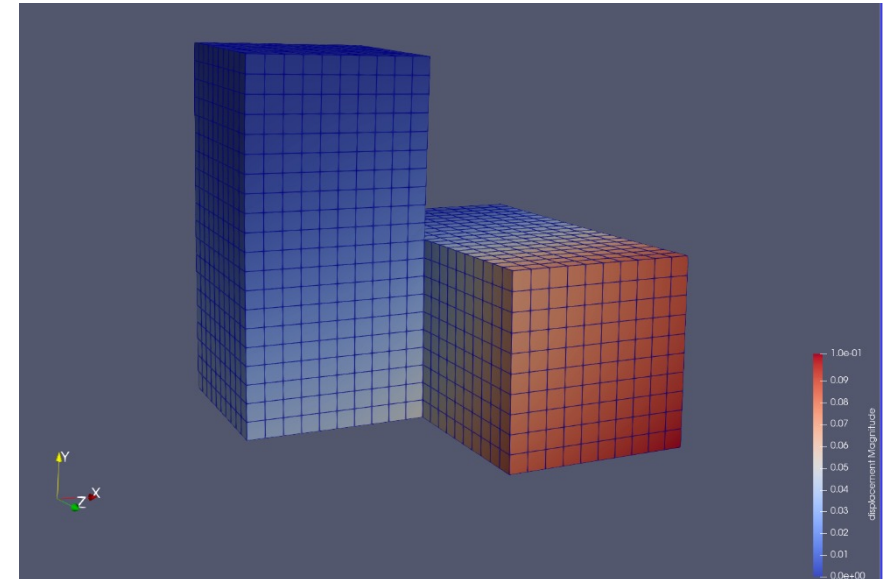
AMGX now included in devel branch

Thomas Zwinger



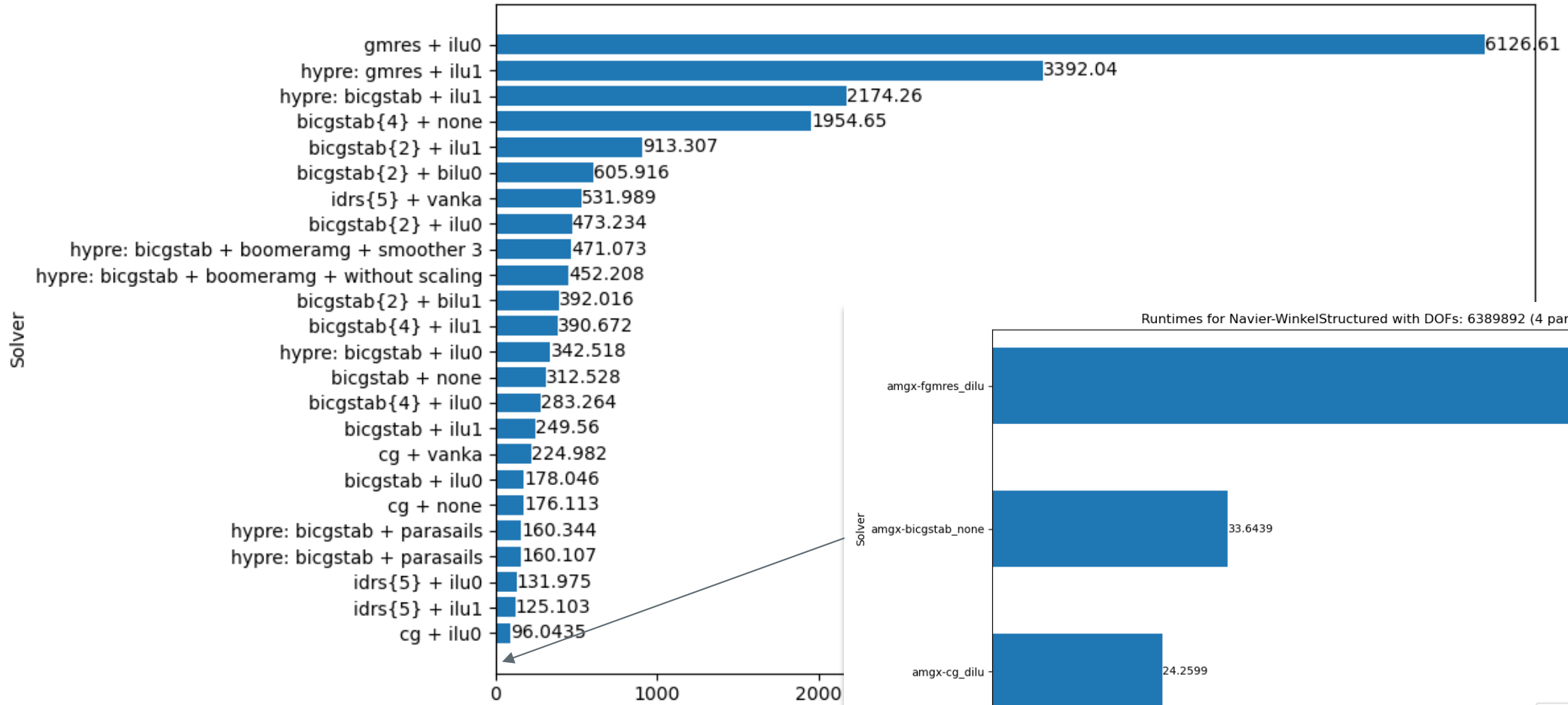
AMGX now included in devel branch

- Tested systematically
<https://github.com/ElmerCSC/elmer-linsys>
- Navier problem on slightly more complex geometry
- Tests on mahti.csc.fi (1 node has 2x64 cores AMD Rome and 4 Nvidia Ampere A100 GPUs)
- Compared to tests on CPU-only nodes

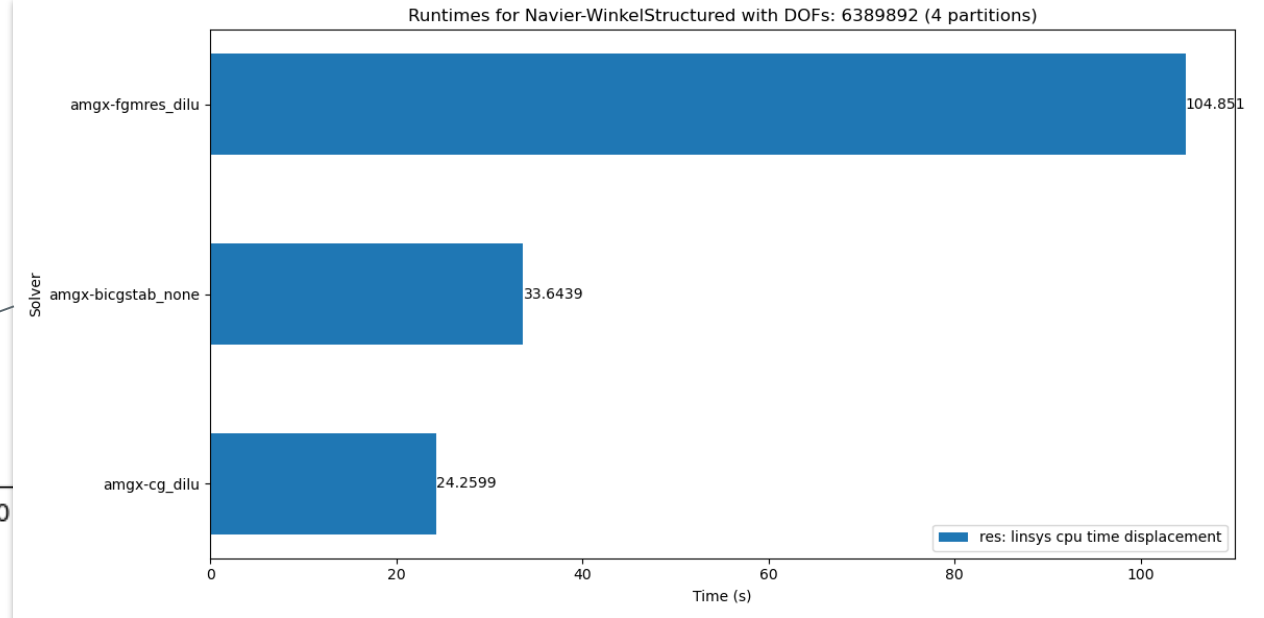


AMGX performance

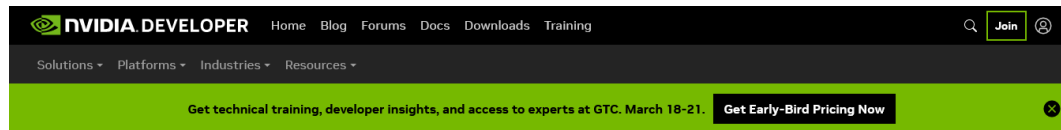
Runtimes for Navier-WinkelStructured with DOFs: 7095876 (128 partitions)



Runtimes for Navier-WinkelStructured with DOFs: 6389892 (4 partitions)



<https://developer.nvidia.com/amgx>



AmgX

AmgX provides a simple path to accelerated core solver technology on NVIDIA GPUs. AmgX provides up to 10x acceleration to the computationally intense linear solver portion of simulations, and is especially well suited for implicit unstructured methods.

It is a high performance, state-of-the-art library and includes a flexible solver composition system that allows a user to easily construct complex nested solvers and preconditioners.



Check out these case studies and white papers:

- ▶ AmgX: Multi-Grid Accelerated Linear Solvers for Industrial Applications
- ▶ AmgX V1.0: Enabling Reservoir Simulation with Classical AMG
- ▶ AmgX: A Library for GPU Accelerated Algebraic Multigrid and Preconditioned Iterative Methods

Get Started with AmgX Today

The AmgX library offers optimized methods for massive parallelism, the flexibility to choose how the solvers are constructed, and is accessible through a simple C API that abstracts the parallelism and GPU implementation.

Using the methods and tools from the AmgX library, developers can easily create specialized solvers using AmgX core methods and rapidly deploy solution on GPU workstations, servers and clusters.

Key Features

- ▶ Flexible configuration allows for nested solvers, smoothers, and preconditioners
- ▶ Ruge-Steuben algebraic multigrid
- ▶ Un-smoothed aggregation algebraic multigrid
- ▶ Krylov methods: PCG, GMRES, BICGSTab, and flexible variants
- ▶ Smoothers: Block-Jacobi, Gauss-Seidel, incomplete LU, Polynomial, dense LU
- ▶ Scalar or coupled block systems
- ▶ MPI support
- ▶ OpenMP support
- ▶ Flexible and simple high level C API

- Anyone with an Nvidia card (also consumer) can use it

- Downloadable under

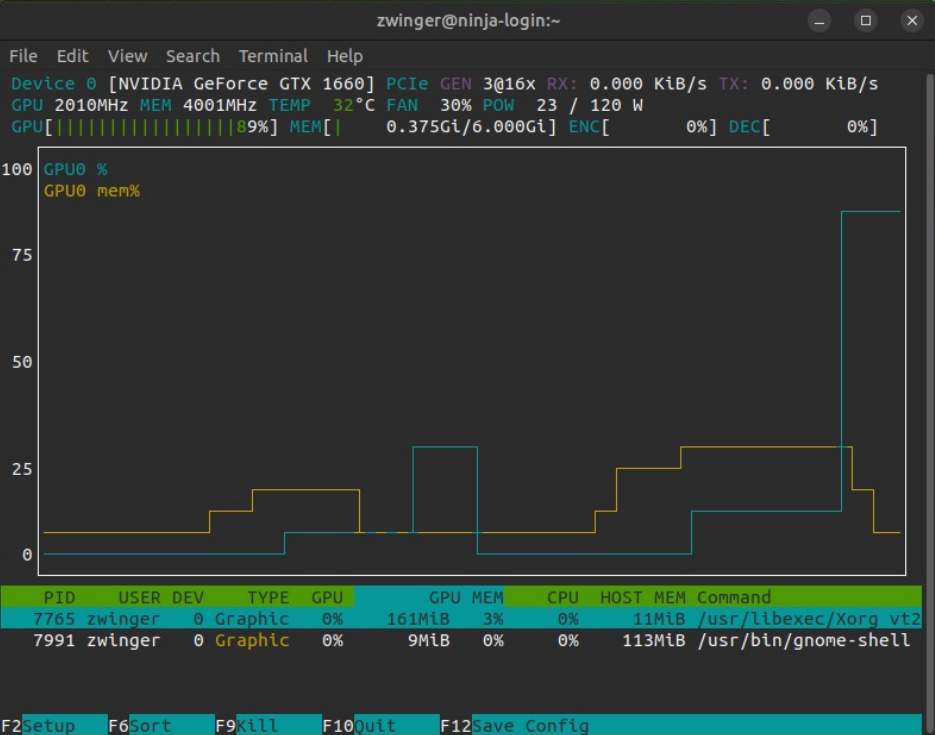
<https://github.com/NVIDIA/AMGX>

- Test: WinkelBmPoissonAMGX

- Needs special cmake flags

```
-DWITH_AMGX:BOOL=TRUE \
-DAMGX_ROOT="${AMGX_HOME}" \
-DAMGX_INCLUDE_DIR="${AMGX_HOME}/include/;${CUDAINC}" \
-DAMGX_LIBRARY="${AMGX_HOME}/lib/libamgx.a" \
-DCUDA_LIBRARIES="-L${CUDALIB} -lcusparse -lcublas -lcusolver -lculat_static -
InvToolsExt -ldl -lpthread /usr/lib64/librt.so" \
-DCUDA_LIBDIR="${CUDALIB}" \
-DCUDA_INCLUDE_DIR="${CUDAINC}" \
```

AMGX ctest testcase



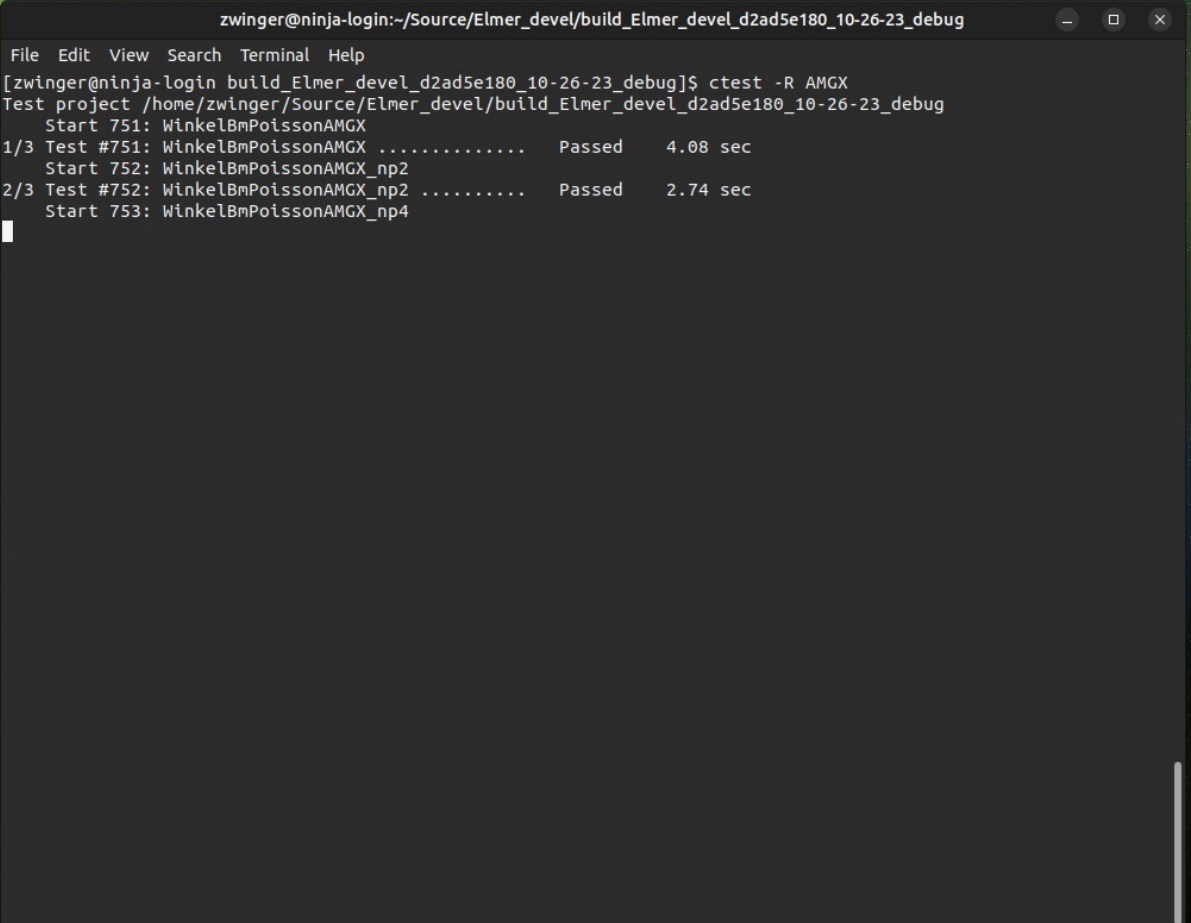
zwinger@ninja-login:~

```
File Edit View Search Terminal Help
Device 0 [NVIDIA GeForce GTX 1660] PCIe GEN 3@16x RX: 0.000 KiB/s TX: 0.000 KiB/s
GPU 2010MHz MEM 4001MHz TEMP 32°C FAN 30% POW 23 / 120 W
GPU[|||||||||||||09%] MEM[ 0.375Gi/6.000Gi] ENC[ 0%] DEC[ 0%]
```

100 GPU0 %
GPU0 mem%

PID	USER	DEV	TYPE	GPU	GPU MEM	CPU	HOST MEM	Command
7765	zwinger	0	Graphic	0%	161MiB 3%	0%	11MiB	/usr/libexec/Xorg vt2
7991	zwinger	0	Graphic	0%	9MiB 0%	0%	113MiB	/usr/bin/gnome-shell

F2Setup F6Sort F9Kill F10Quit F12Save Config



zwinger@ninja-login:~/Source/Elmer_devel/build_Elmer_devel_d2ad5e180_10-26-23_debug

```
File Edit View Search Terminal Help
[zwinger@ninja-login build_Elmer_devel_d2ad5e180_10-26-23_debug]$ ctest -R AMGX
Test project /home/zwinger/Source/Elmer_devel/build_Elmer_devel_d2ad5e180_10-26-23_debug
Start 751: WinkelBmPoissonAMGX
1/3 Test #751: WinkelBmPoissonAMGX ..... Passed 4.08 sec
Start 752: WinkelBmPoissonAMGX_np2
2/3 Test #752: WinkelBmPoissonAMGX_np2 ..... Passed 2.74 sec
Start 753: WinkelBmPoissonAMGX_np4
```

Elmer GPU developments

- Porting to AMD world (ROCalution instead of AMGX)
- Started looking into OpenMP GPU offloading for matrix assembly (this is hard)
- Currently issues with data transfer between main and GPU memory - might go away with next gen hardware
- Final goal is that main Elmer/Ice solvers at some stage run on GPUs

Reporting unused keywords

- Ease of adding keywords in Elmer has a caveat
 - You can easily add unused keywords without realizing that they have no effect
- Typos may go unnoticed when casting
- Copy-pasting leaves history of previous sif file
- Not all keywords are futile, they just where not needed this time...

MAIN: Reporting unused list entries for sif improvement!

MAIN: If you do not want these lines undefine > DEVEL_LISTUSAGE < !

Unused keywords:

Simulation	debug element
Constants	stefan boltzmann
Boundary Condition 2	velocity 1
Boundary Condition 2	velocity 2
Boundary Condition 2	velocity 3
Solver 2	flow model
Solver 2	linear system abort not converged
Solver 2	viscosity newton relaxation factor
Solver 2	nonlinear system consistent norm

MAIN: *** Elmer Solver: ALL DONE ***

Report unused keywords

- Activation & deactivation in fem/config.h.cmake
- + "Max Output Level >= 6"

```
/* Have these defined only for debugging or optimization purposes */  
/* #define DEVEL_LISTCOUNTER */  
#define DEVEL_LISTUSAGE  
/* #define DEVEL_KEYWORDMISSES */
```


Unused keywords:

```
Simulation      debug element
Simulation      solver input file
Simulation      timer: loadmesh real time
Simulation      timer: meshstabparams real time
Simulation      initialization phase
Constants       stefan boltzmann
Boundary Condition 1 name
Boundary Condition 2 name
Boundary Condition 2 velocity 1
Boundary Condition 2 velocity 2
Boundary Condition 2 velocity 3
Material 1      name
Solver 1        active mesh dimension
Solver 1        no matrix
Solver 2        flow model
Solver 2        linear system abort not converged
Solver 2        viscosity newton relaxation factor
Solver 2        nonlinear system consistent norm
Solver 2        active mesh dimension
Solver 3        active mesh dimension
```

Used keywords:

```
Simulation      2      coordinate system
Simulation      7      simulation type
Simulation      1      steady state max iterations
Simulation      1      steady state min iterations
Simulation      1      initialize dirichlet conditions
Simulation      1      max output level
Simulation      2      extruded mesh levels
Simulation      1      extruded max coordinate
Constants       2      gas constant
Constants       1      gravity
Equation 1     3      active solvers
Equation 1     3      mapcoordinate
Equation 1     6      hydro-stokes
Equation 1     3      resultoutput
Body Force 1   4      flow bodyforce 1
```

```
Body Force 1   4      flow bodyforce 2
Body Force 1   4      flow bodyforce 3
Boundary Condition 1 5      target boundaries
Boundary Condition 2 13139 bottom surface
Boundary Condition 2 78836 horizvelo 1
Boundary Condition 2 78836 horizvelo 2
Boundary Condition 3 13140 top surface
Material 1     5      density
Material 1     4      viscosity
Material 1     4      viscosity model
Material 1     3      glen exponent
Material 1     3      critical shear rate
Material 1     2      limit temperature
Material 1     2      rate factor 1
Material 1     2      rate factor 2
Material 1     2      activation energy 1
Material 1     2      activation energy 2
Material 1     2      glen enhancement factor
Material 1     2      set arrhenius factor
Material 1     3      arrhenius factor
Solver 1       4      exec solver
Solver 1       9      equation
Solver 1       4      procedure
Solver 1       1      active coordinate
Solver 1       1      mesh velocity variable
Solver 1       1      mesh velocity first zero
Solver 1       1      dot product tolerance
Solver 2      16      equation
Solver 2       4      procedure
Solver 2       2      variable
Solver 2       1      optimize bandwidth
Solver 2       8      linear system solver
Solver 2       2      linear system iterative me
Solver 2       2      linear system max iteratio
Solver 2       3      linear system residual out
Solver 2       2      linear system convergence
Solver 2       5      linear system precondition
Solver 2       2      nonlinear system max ite
```

HydrostaticNSVec



- Ref: Ralf Greve & Heinz Blatter: *Dynamics of Ice Sheets and Glaciers*
- Motivation
 - Missing piece between full 3D Stokes (IncompressibleNSVec) and 2D shell solvers
 - Much smaller linear system compared to full Stokes 2x2 vs 4x4
 - Pos.def. linear system - Not a saddle-point problem
=> large selection of good linear system strategies!?
- Implementation strategy
 - Copy-paste from IncompressibleNSVec
 - Use of same keywords as much as possible
 - Pre/post processing automated via internal use of structured mesh
- Additional assumption
 - 3D mesh with generated via extrusion

HydrostaticNSVec – the model

- Hydrostatic 1st order approximation

$$\frac{\partial v_z}{\partial x} / \frac{\partial v_x}{\partial z}, \quad \frac{\partial v_z}{\partial y} / \frac{\partial v_y}{\partial z} \sim \frac{[W]}{[L]} / \frac{[U]}{[H]} = \frac{[W]}{[U]} \frac{[H]}{[L]} = \varepsilon^2 \sim 10^{-6}$$

G&B (5.68)

- Resulting to:

$$\begin{aligned}
 &4 \frac{\partial}{\partial x} \left(\eta \frac{\partial v_x}{\partial x} \right) + 2 \frac{\partial}{\partial x} \left(\eta \frac{\partial v_y}{\partial y} \right) + \frac{\partial}{\partial y} \left(\eta \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) \right) \\
 &\quad + \frac{\partial}{\partial z} \left(\eta \frac{\partial v_x}{\partial z} \right) = \rho g \frac{\partial h}{\partial x}, \\
 &4 \frac{\partial}{\partial y} \left(\eta \frac{\partial v_y}{\partial y} \right) + 2 \frac{\partial}{\partial y} \left(\eta \frac{\partial v_x}{\partial x} \right) + \frac{\partial}{\partial x} \left(\eta \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) \right) \\
 &\quad + \frac{\partial}{\partial z} \left(\eta \frac{\partial v_y}{\partial z} \right) = \rho g \frac{\partial h}{\partial y}.
 \end{aligned}$$

Elliptic operators
Diagonally dominated
2x2 block system

Easy!

G&B (5.70)

Nonlinear viscosity

- Nonlinear viscosity model exactly as in IncompressibleNSVec with strainrate velocity defined by

$$d_e = \left\{ \left(\frac{\partial v_x}{\partial x} \right)^2 + \left(\frac{\partial v_y}{\partial y} \right)^2 + \frac{\partial v_x}{\partial x} \frac{\partial v_y}{\partial y} + \frac{1}{2} \frac{\partial v_x}{\partial y} \frac{\partial v_y}{\partial x} + \frac{1}{4} \left(\frac{\partial v_x}{\partial y} \right)^2 + \frac{1}{4} \left(\frac{\partial v_y}{\partial x} \right)^2 + \frac{1}{4} \left(\frac{\partial v_x}{\partial z} \right)^2 + \frac{1}{4} \left(\frac{\partial v_y}{\partial z} \right)^2 \right\}^{1/2}$$

G&B (5.71)

Postprocessing fields

- Vertical velocity

$$v_z = v_z|_{z=b} - \int_b^z \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} \right) d\bar{z} .$$

G&B (5.72)

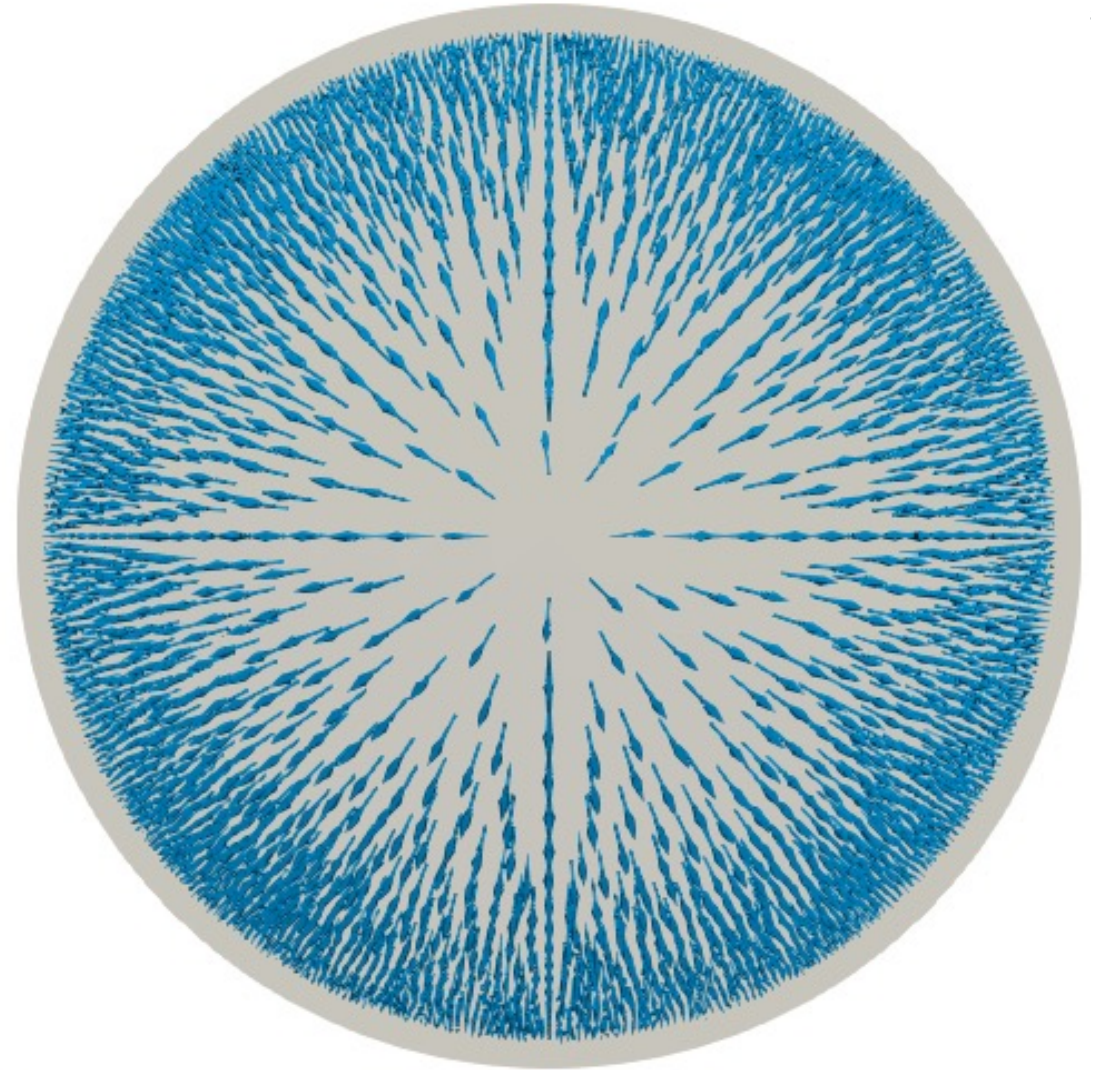
$$\cancel{\frac{\partial b}{\partial t}} + v_x \frac{\partial b}{\partial x} + v_y \frac{\partial b}{\partial y} - v_z = N_b \cancel{c_b^T} .$$

G&B (5.31)

- Derivatives appearing in postprocessing are averaged over elements!

HydrostaticNSVec: Buehler profile

- This case should be straight-forward
- How to estimate the error?
- New operators for StructuredProjectToPlane
 - "error norm"
 - "error max"
 - "error projected"



HydrostaticNSVec: Buehler profile

Solver 4

Equation = "ModelError"

Procedure = "StructuredProjectToPlane"

"StructuredProjectToPlane"

Active Coordinate = Integer 3

Project to everywhere = Logical True

Variable 1 = HorizVelo

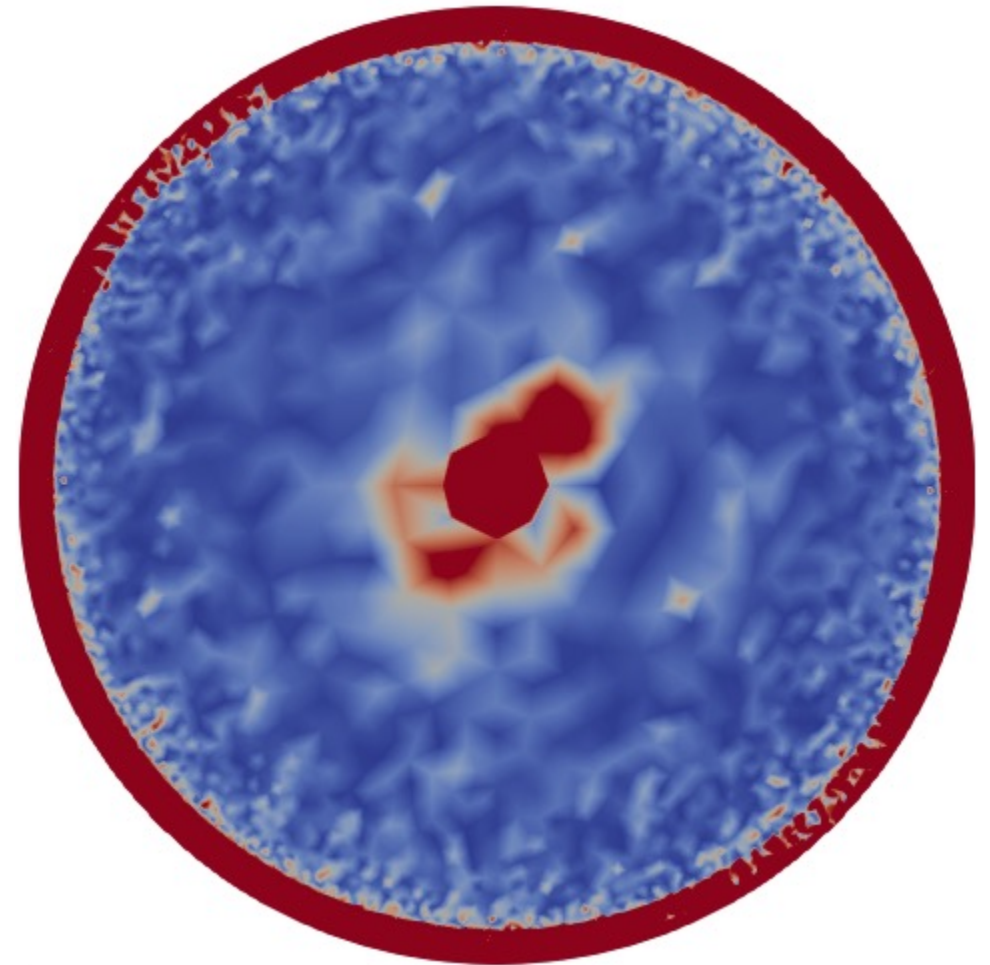
Error Variable 1 = String "Flow Solution"

Operator 1 = "error norm"

Target Variable 1 = "velo error"

End

$$err = |u - v| / (|u| + |v|) / 2$$



Error scaled to [0,0.001]

HydrostaticNSVec: Buehler profile

Solver 4

Equation = "ModelError"

Procedure = "StructuredProjectToPlane"

"StructuredProjectToPlane"

Active Coordinate = Integer 3

Project to everywhere = Logical True

Variable 1 = HorizVelo

Error Variable 1 = String "Flow Solution"

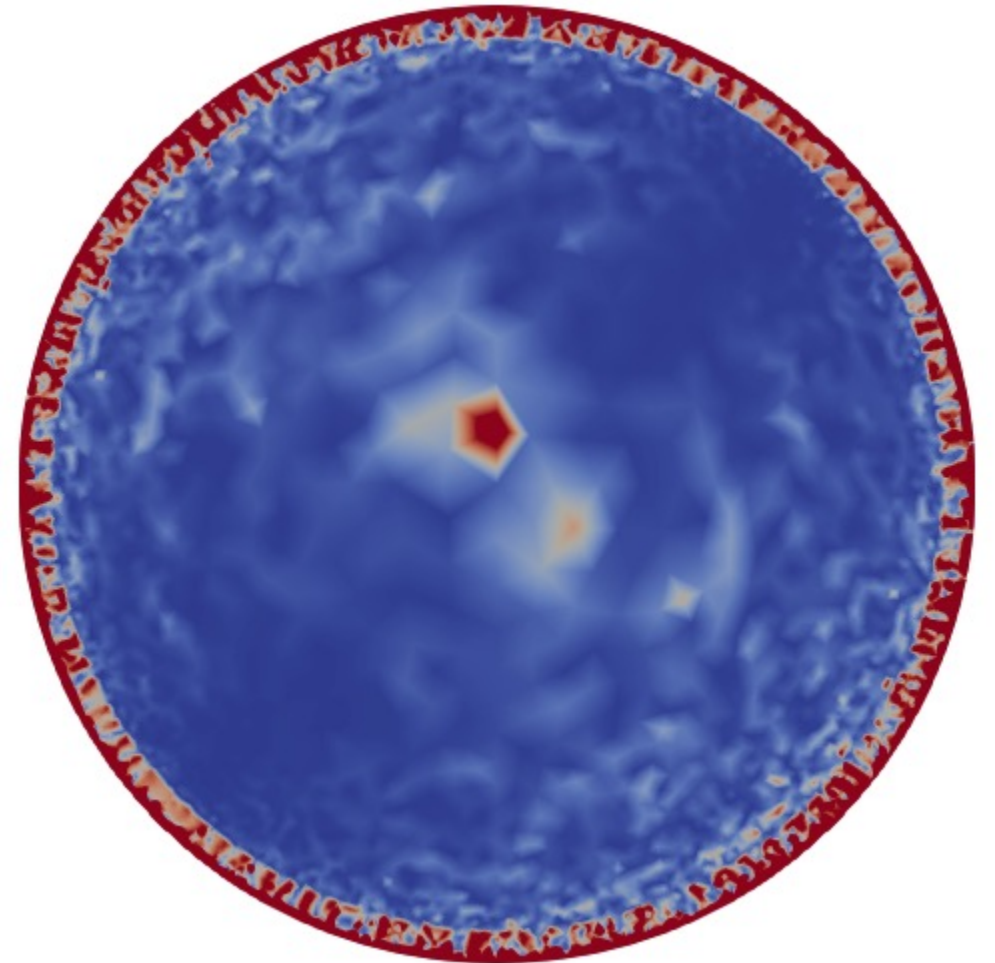
Operator 1 = "error projected"

Target Variable 1 = "velo projected error"

End

Find c that minimizes $|u - cv|$!

$$err = |u - cv| / (|u| + |cv|) / 2$$



Error scaled to [0,0.001]

HydrostaticNSVec: Buehler profile

Solver 4

```
Equation = "ModelError"
```

```
Procedure = "StructuredProjectToPlane"
```

```
"StructuredProjectToPlane"
```

```
Active Coordinate = Integer 3
```

```
Project to everywhere = Logical True
```

```
Variable 1 = HorizVelo
```

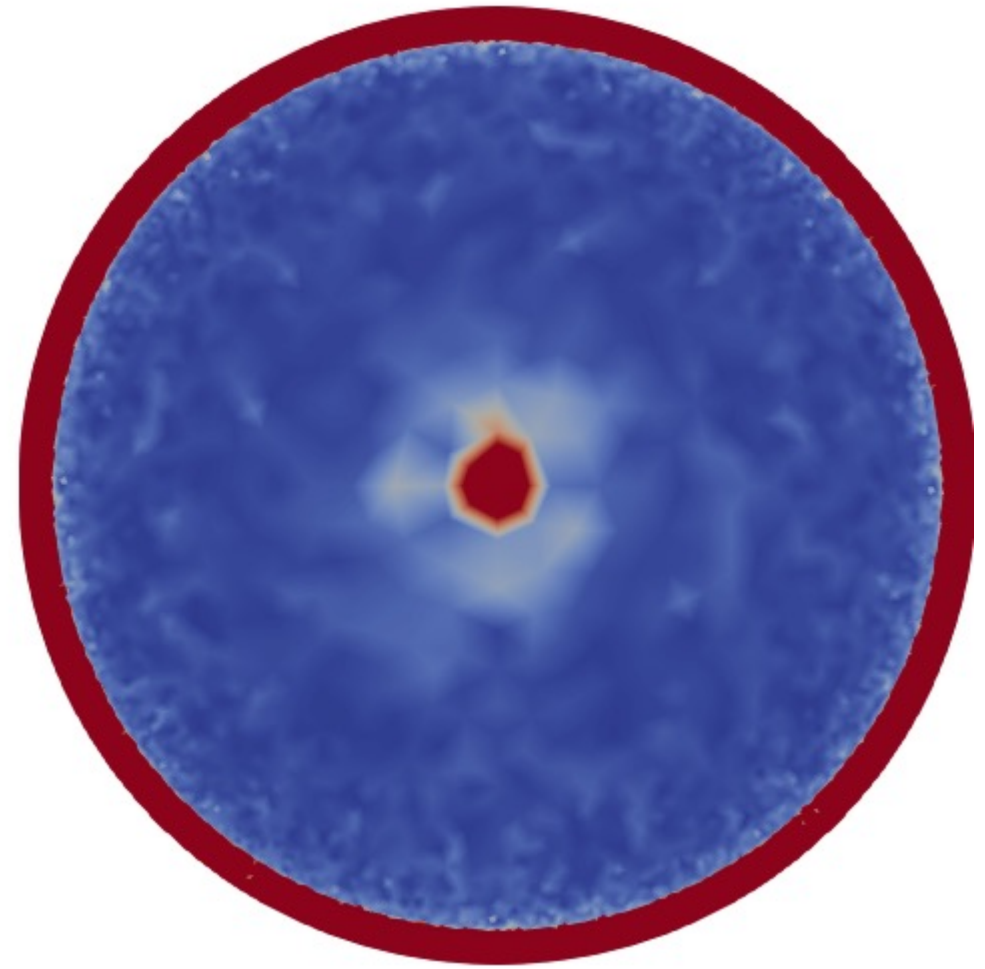
```
Error Variable 1 = String "Flow Solution"
```

```
Operator 1 = "error max"
```

```
Target Variable 1 = "velo error max"
```

```
End
```

$$err = |u - v|_{\infty} / (|u|_{\infty} + |v|_{\infty}) / 2$$



Error scaled to [0,0.001]

HydrostaticNSVec – initial guess for 3D Stokes

- We can run the two solvers in sequence
- Does this help in convergence?
- A simple case with Picard was studied
 - “Constant-Viscosity Start = False”
- We may be able to replace more expensive iterations with cheaper ones
 - Effect is not dramatic even at best
- Might save initial convergence?

Relative error with combined iteration count



HydrostaticNSVec – using simpler model as preconditioner?

- For 3D Stokes: $Au=b$
- For Hydrostatic Stokes: $Bv=c$
- GCR sequence for $Au=b$
 - Compute $r=Au-b$
 - Project r to c
 - Solve $Bv=c$
 - expand v to dx
- Preliminary machinery in Elmer (for other problems)
- probably does not beat the block preconditioner...

HydrostaticNSVec – consistency test

- ISMIP HOM C

