Elmer/Ice Course - MLB

CSC



Spitzbergen

SVALBARD

Vestfonna

Austfonna

https://wgms.ch/products_ref_glaciers/midtre -lovenbreen-svalbard/

Reconstructing Climate: Midtre Lovénbreen, Svalbard



Pictures and data provided by Jack Kohler, NPI, NOR (2005 DEM from NERC)

- DEM's obtained at different times
- Using 2 consecutive time-levels
 - Obtaining averaged DEM

$$\circ \qquad \qquad h_{2000} = (h_{2005} - h_{1995})/2$$

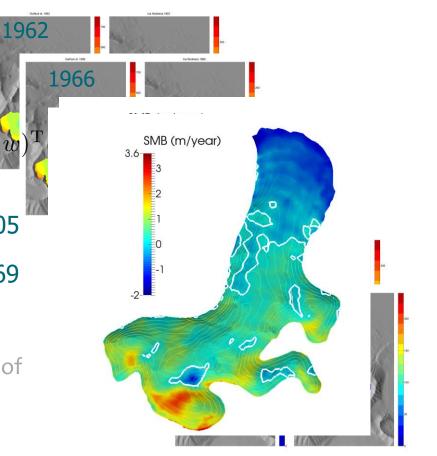
• and local elevation change

 $\frac{\partial h}{\partial t}|_{2000} = (h_{2005} - h_{1995})/11$

- Elmer/Ice full Stokes diagnostic simulations $\rightarrow u = (u, v, w)$
- Spatial distribution of SMB:

$$SMB = \left(\frac{\partial h}{\partial t} + u\frac{\partial h}{\partial x} + v\frac{\partial h}{\partial y} - w\right)$$

Välisuo, I., T. Zwinger and J. Kohler (2017): **Inverse solution of surface mass balance of Midtre Lovénbreen, Svalbard**, Journal of Glaciology, 1-10, doi:10.1017/jog.2017.26.

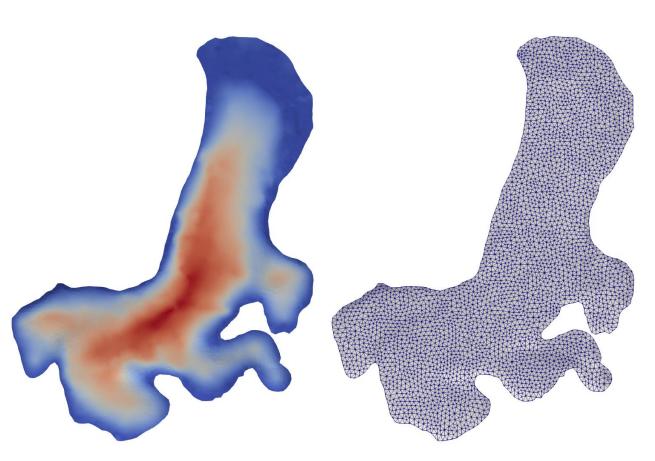


1995-2005

1962-1969

This exercise

- We take the DEM of 1995
- We will run a diagnostic simulation on the given geometry
- Emphasis on some special features
 - $\circ_3 D$ mesh generation using extrusion
 - \circ Restart from 2D data
 - $\circ\mbox{Utilizing}$ extruded structure in mesh deformation
 - Vectorized & threaded version of Navier-Stokes
 - Block preconditioning
 - Semilagrangian solver for purely convective transport i.e. of age
- Users are free to try out different things
 - \circ Solution strategies
 - o Parallel runs

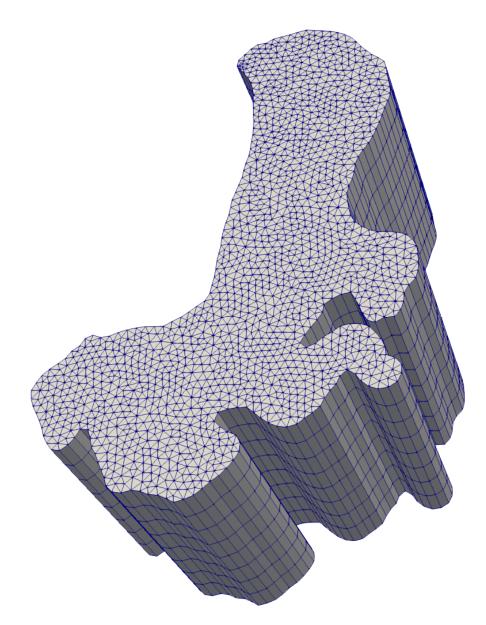


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Finalizing mesh using internal extrusion

- The mesh is finalized in memory starting from 2D footprint
- Here the extruded height does not play any role • Mesh is further adapted to follow true bottom and top

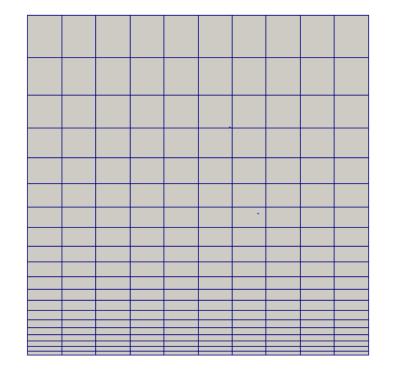
```
Simulation
Extruded Mesh Levels = Integer 9
Extruded Max Coordinate = Real 1000
```



Internal mesh extrusion

- Start from an initial 2D (1D) mesh and then extrude into 3D (2D)
 Mesh density may be given a geometric ratio and even an arbitrary function
- Implemented also for partitioned meshes

 Extruded lines belong to the same partition by construction!
- Effectively eliminates meshing bottle-necks
- Side boundaries get a BC constraint so that o2D constraint BC = 1D contraint BC + offset ooffset is set if the baseline BCs are preserved
- Top and bottom boundaries get the next free BC constraint indexes
 - oNote thet the BCs refer directly to the "Boundary Condition"
 - "Target Boundaries" is used only when reading in the mesh in the 1st place and they are not available any more at this stage



Extruded Mesh Levels = 21
Extruded Mesh Density =
 Variable Coordinate 1
 Real MATC "1+10*tx"

Restart from 2D data: Mesh2MeshSolver

- We can take 2D data and interpolate it to top/bottom layers of 3D mesh o2D interpolatio task with z-coordinate neglected
- Makes workflow easier since the data needs to be interpolated only once to an Elmer mesh
- 2D file is read in full to all processes • Same restart file can be used for any number of cores!
- We have precomputed restart files for you!

```
Solver 1
Exec Solver = before all
Equation = "InterpSolver"
Procedure = "Mesh2MeshSolver" "Mesh2MeshSolver"
```

! Restart is here always from a serial mesh
Mesh = -single \$restartdir
Restart File = \$restartfile

! We use the primary 2D mesh with local copy Mesh Enforce Local Copy = Logical True

```
! These are the variables for restart
Restart Position = Integer 0
Restart Variable 1 = String "bedrockDEM"
Restart Variable 2 = String "surfaceDEM1995"
```

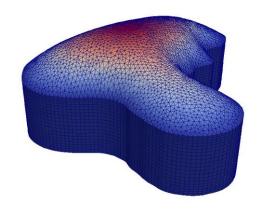
! Ensures that we perform interpolation on plane Interpolation Passive Coordinate = Integer 3 End

Utilizing extruded structure in mesh deformation: StructuredMeshMapper



- The shape of the mesh needs to be accomodated
 - \circ Bottom of ice follows bedrock
 - $\circ \mathsf{Top}$ of ice follows ice surface
- This could be done using generic 3D techniques

 MeshSolve (version of linear elasticity equation)
 Expensive and unnecessary!
- We can apply to each extruded node 1D mapping • Very cheap!



```
! Maps the constant-thickness mesh
! between given bedrock and surface topology
Solver 2
  Exec Solver = "before simulation"
  Equation = "MapCoordinate"
  Procedure = "StructuredMeshMapper" "StructuredMeshMappe
```

```
Active Coordinate = Integer 3
Displacement Mode = Logical False
Correct Surface = Logical True
Minimum Height = Real 5.0
Correct Surface Mask = String "Glaciated"
Dot Product Tolerance = 1.0e-3
```

```
! Allocate some fields here
Variable = MeshUpdate
Exported Variable 1 = "bedrockDEM"
Exported Variable 1 Mask = String "BedRock"
Exported Variable 2 = "surfaceDEM1995"
Exported Variable 2 Mask = String "Surface"
End
```

Using extruded structure for mapping: StructuredProjectToPlane



• We may perform various operations along the extruded 1D lines

Computation of height & depth

oComputation of integrals over the depth etc.

```
! Computes height and depth assuming an
! extruded mesh.
Solver 3
  Exec Solver = "before simulation"
  Equation = "HeightDepth"
  Procedure = "StructuredProjectToPlane"
"StructuredProjectToPlane"
  Active Coordinate = Integer 3
  Operator 1 = depth
  Operator 2 = height
End
```

New Stokes solver: IncompressibleNSVec

• FlowSolve is one of the oldest modules in Elmer

○Has a lot of extra baggage

oCannot ideally utilize modern CPU architectures

• IncompressibleNSVec is fresh out of the oven

oIncludes vectorization and threading

oTakes use of code modernination in many places

 OUnfortunately vectorization and threading do not make the modules prettier

• Performance boost depends heavily on the length of the vectors

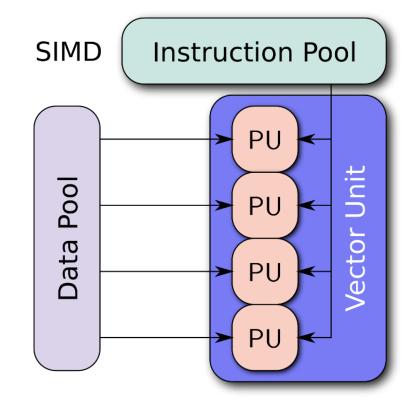
 $\circ \text{Number of Gaussian integration points}$

🔒 IncompressibleNSVec.F90 - emacs dBasisdxVec(1:ngp,1:ntot,i), dBasisdxVec(1:ngp,1:ntot,j), weight c, stif ford(1:ntot,1:ntot,i,j)) END DO END DO END IF IF (GradPVersion) THEN ! b(u,q) = (u, qrad q) partDO i = 1, dimCALL LinearForms UdotV(ngp, ntot, elemdim, & BasisVec, dbasisdxvec(:,:,i), detJVec, stifford(:,:,i,dofs)) StiffOrd(:,:,dofs,i) = transpose(stifford(:,:,i,dofs)) END DO ELSE DO i = 1, dim CALL LinearForms UdotV(ngp, ntot, elemdim, & dBasisdxVec(:, :, i), BasisVec, -detJVec, StiffOrd(:,:,i,dofs)) StiffOrd(:,:,dofs,i) = transpose(stifford(:,:,i,dofs)) END DO END IF ! Masses (use symmetry) ! Compute bilinear form G=G+(alpha u, u) = u .dot. (grad u) IF (.NOT. StokesFlow) THEN CALL LinearForms UdotU(ngp, ntot, elemdim, BasisVec, DetJVec, VelocityMass, rhov ₽ ¶ec) ! Scatter to the usual local mass matrix DO i = 1, dim mass(i::dofs, i::dofs) = mass(i::dofs, i::dofs) + VelocityMass(1:ntot, 1:ntot) END DO !CALL LinearForms UdotU(ngp, ntot, elemdim, BasisVec, DetJVec, PressureMass, -ka sppavec) !mass(dofs::dofs, dofs::dofs) = mass(dofs::dofs, dofs::dofs) + PressureMass(1:nt) sot,1:ntot) U:--- IncompressibleNSVec.F90 28% L370 Git-devel (F90 AC Abbrev

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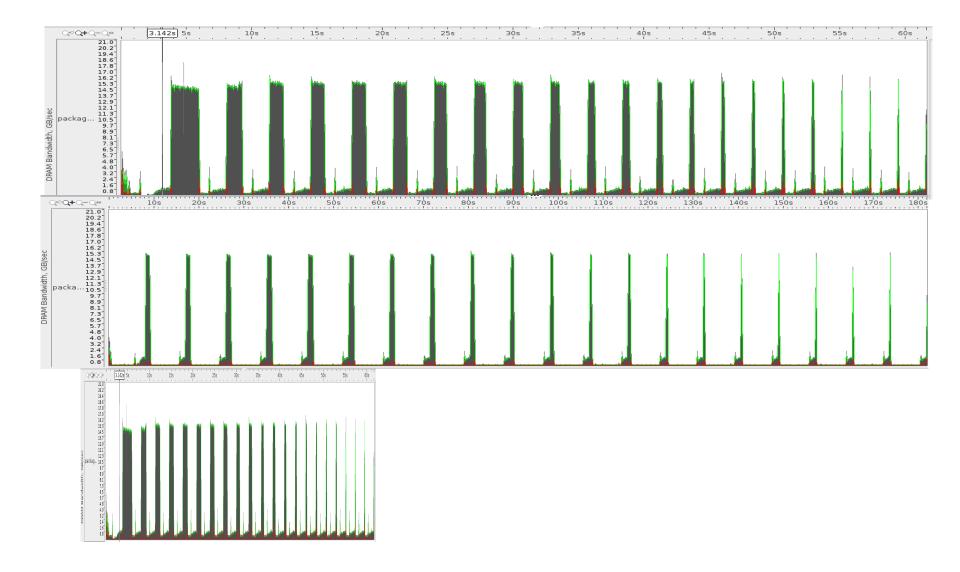
Motivation for new Stokes Solver

- New computer architectures use SIMD (=vector) units to do fast computations
- If you (on an Intel chip) don't utilize this, you a priori loose ³/₄ of your performance
- FEM: assembly = creating the matrix solution = solving it
- Until recently, assembly procedures in Elmer did not utilize SIMD
- New Stokes solver does!
- Gains depend on the number of integration points



By Vadikus - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=39715273 csc

Comparison vectorised/legacy Solver using Intel VTune





Using the new Stokes Solver

- We have to specify that this is a Stokes model olnertia terms neglected
- We can start with constant viscosity • Eliminates need for initial guess
- Number of integration points affects the accuracy of discretization

 \circ Has significant effect on performance!

- We may use different solution techniques for linear solver
 - \circ Iterative method

 $\circ \text{Direct metod}$

 \circ Block preconditioning (next topic)

- Nonlinear solver takes use of Newton's linearization
 - Started with Picard iteration that has larger radius of convergence

Solver 4
Equation = "Stokes-Vec"
Procedure = "IncompressibleNSVec" "IncompressibleNSSolver"
Flow Model = Stokes

```
! 1st iteration viscosity is constant
Constant-Viscosity Start = Logical True
```

! Accuracy of numerical integration (on wedges)
Number of Integration Points = Integer 44 ! 21, 28, 44, 64, ...

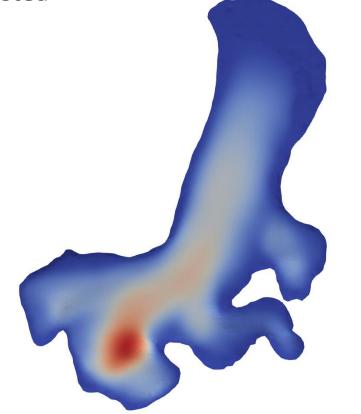
```
! Iterative approach:
Linear System Solver = Iterative
Linear System Iterative Method = "GCR"
Linear System Max Iterations = 500
Linear System Convergence Tolerance = 1.0E-08
Linear System Abort Not Converged = False
Linear System Preconditioning = "ILU1"
Linear System Residual Output = 10
```

```
! Direct approach (as alternative to above):
!Linear System Solver = Direct
!Linear System Direct Method = MUMPS
```

```
!Non-linear iteration settings:
Nonlinear System Max Iterations = 50
Nonlinear System Convergence Tolerance = 1.0e-5
Nonlinear System Newton After Iterations = 10
Nonlinear System Newton After Tolerance = 1.0e-1
Nonlinear System Consistent Norm = True
! Nonlinear System Relaxation Factor = 1.00
```

Material law for Ice

- Ice is a shear-thinning fluid and requires a complicated viscosity model
- Plain viscosity is used in the 1st solution if requested



```
Material 1
Name = "Ice"
Density = Real $rhoi
```

! First viscosity with newtonian fluid ! happens to give velocities of proper size Viscosity = Real 1.0

```
! Nonnewtonian viscosity
Viscosity Model = String Glen
Glen Exponent = Real 3.0
Critical Shear Rate = Real 1.0E-10
! Paterson value in MPa^-3a^-1
Limit Temperature = Real -10.0
Rate Factor 1 = Real $A1
Rate Factor 2 = Real $A2
Activation Energy 1 = Real $Q1
Activation Energy 2 = Real $Q2
Glen Enhancement Factor = Real 1.0
Relative Temperature = Real $Tc
End
```



Block preconditioning

- In parallel runs a central challenge is to have good **parallel preconditioners**
- This problem is increasingly difficult for PDEs with vector fields Navier-Stokes, elasticity, acoustics,...
 Strongly coupled multiphysics problems
- Preconditioner need not to be just a matrix, it can be a procedure!
- Idea: Use as preconditioner a procedure where the components are solved one-by-one and the solution is used as a **search direction** in an outer Krylov method
- Number of outer iterations may be shown to be bounded
- Individual blocks may be solved with optimally scaling methods oMultilevel methods

Preconditioner (from right):

Instead of solving

 $\mathbf{K}\mathbf{x} = \mathbf{b}$

Identify a preconditioner P which makes solution of $\mathbf{K} \mathbf{P}^{-1} \mathbf{z} = \mathbf{b},$

with z=Px easier than the original problem.



Block precontioning

• Given a block system

$$\begin{bmatrix} \mathbf{K}_{11} & \cdots & \mathbf{K}_{1N} \\ & \ddots & \\ \mathbf{K}_{N1} & \cdots & \mathbf{K}_{NN} \end{bmatrix} \begin{bmatrix} \mathbf{x}_{1} \\ \vdots \\ \mathbf{x}_{N} \end{bmatrix} = \begin{bmatrix} \mathbf{b}_{1} \\ \vdots \\ \mathbf{b}_{N} \end{bmatrix}$$
• Block Gauss-Seidel Block Jacobi
$$P = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{0} & \mathbf{0} & \cdots \\ \mathbf{K}_{21} & \mathbf{K}_{22} & \mathbf{0} & \cdots \\ \cdots & & & \end{bmatrix} \qquad P = \begin{bmatrix} \mathbf{K}_{11} & \mathbf{0} & \mathbf{0} & \cdots \\ \mathbf{0} & \mathbf{K}_{22} & \mathbf{0} & \cdots \\ \cdots & & & & \end{bmatrix}$$

CSO

- Preconditioner is the operator which produces the new search direction $s^{\left(k\right)}$
- Use GCR to minimize the residual over the space

$$||\mathbf{b} - \mathbf{K}\mathbf{x}^{(k)}||$$
$$\mathcal{V}_k = \mathbf{x}^{(0)} + \operatorname{span}\{\mathbf{s}^{(1)}, \mathbf{s}^{(2)}, \dots, \mathbf{s}^{(k)}\}$$

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GCR with general search directions to solve Ku = f

$$\begin{split} &k = 0 \\ \mathbf{r}^{(k)} = \mathbf{f} - \mathbf{K} \mathbf{u}^{(k)} \\ &\text{while } (\|\mathbf{r}^{(k)}\| < TOL \|\mathbf{f}\| \text{ and } k < m) \\ &\text{ Generate the search direction } \mathbf{s}^{(k+1)} \\ &\mathbf{v}^{(k+1)} = \mathbf{K} \mathbf{s}^{(k+1)} \\ &\text{ do } j = 1, k \\ &\mathbf{v}^{(k+1)} = \mathbf{v}^{(k+1)} - \langle \mathbf{v}^{(j)}, \mathbf{v}^{(k+1)} \rangle \mathbf{v}^{(j)} \\ &\mathbf{s}^{(k+1)} = \mathbf{s}^{(k+1)} - \langle \mathbf{v}^{(j)}, \mathbf{v}^{(k+1)} \rangle \mathbf{s}^{(j)} \\ &\text{ end do } \\ &\mathbf{v}^{(k+1)} = \mathbf{v}^{(k+1)} / \|\mathbf{v}^{(k+1)}\| \\ &\mathbf{s}^{(k+1)} = \mathbf{s}^{(k+1)} / \|\mathbf{v}^{(k+1)}\| \\ &\mathbf{u}^{(k+1)} = \mathbf{u}^{(k)} + \langle \mathbf{v}^{(k+1)}, \mathbf{r}^{(k)} \rangle \mathbf{s}^{(k+1)} \\ &\mathbf{r}^{(k+1)} = \mathbf{r}^{(k)} - \langle \mathbf{v}^{(k+1)}, \mathbf{r}^{(k)} \rangle \mathbf{v}^{(k+1)} \\ &k = k + 1 \end{split}$$

28.10.2019

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Block preconditioner for the Stokes problem

• Each nonlinear step requires solving the Stokes problem

$$\begin{bmatrix} \mathbf{A} & \mathbf{B}^T \\ \mathbf{B} & \mathbf{C} \end{bmatrix} \begin{bmatrix} \mathbf{V} \\ \mathbf{P} \end{bmatrix} = \begin{bmatrix} \mathbf{F} \\ \mathbf{G} \end{bmatrix}$$

 Note that here C is result of stabilization, with suitable choice of basis vectors it can also be zero. The preconditioner is of the form

$$\mathsf{P} = \left[\begin{array}{cc} \mathbf{A} & \mathbf{B}^{\mathcal{T}} \\ \mathbf{0} & \mathbf{Q} \end{array} \right]$$

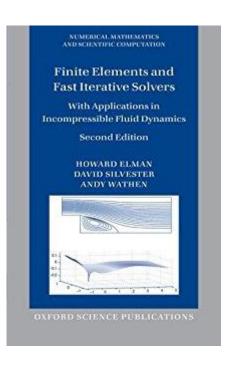
• An optimal choice of Q corresponds to the Schur complement. Usual choice is

 $\mathbf{Q} = \varepsilon^{-1} \mathbf{M},$

where M is the mass matrix and $\boldsymbol{\epsilon}$ is the viscosity from previous iteration.

• We may split A to 3x3 submatrix also, or not

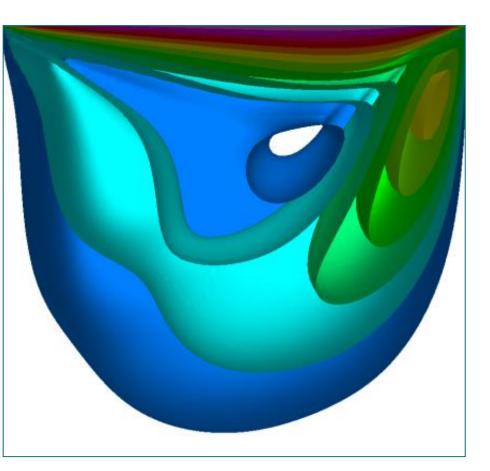
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H. Elman, D. Silvester, A. Wathen, Finite Elements and Fast Iterative Solvers: with Applications in Incompressible Fluid Dynamics, OUP Oxford, 2005.

Block preconditioner: Weak scaling of 3D driven-cavity

Elems	Dofs	#procs	Time (s)
34^3	171,500	16	44.2
43^3	340,736	32	60.3
54^3	665,500	64	66.7
68^3	1,314,036	128	73.6
86^3	2,634,012	256	83.5
108^3	5,180,116	512	102.0
132^3	9,410,548	1024	106.8



Velocity solves with Hypre: CG + BoomerAMG preconditioner for the 3D driven-cavity case (Re=100) on Cray XC (Sisu). Simulation Mika Malinen, CSC, 2013.

0(~1.14)



Using block solver strategy with new Stokes module

- We choose overall block splitting and strategy
- GCR is recommended for outer level • Does not require preconditioner to be exact!
- Different strategies may basically be used for different blocks for each **inner** system
 - \circ Blocks 1,2,3 here associated with velocity components 1,2,3
 - \odot Block 4 associated with pressure (preconditioned with scaled mass matrix is suggested by Elman)
- The strategy recides nowadays almost completely in the library functionality of Elmer
 - Makes dedicated block-preconditioned ParStokes obsolite
 - $\circ\,\mbox{This}$ strategy is not available in FlowSolver
- Note: the benefits of optimal scaling become obvious when the size of the problem grows

! Setting to choose block solver strategy Linear System Solver = "Block" Block Gauss-Seidel = Logical True Block Scaling = Logical False Block Preconditioner = Logical True ! Block Structure(4) = Integer 1 1 1 2 Block Order(4) = Integer 1 2 3 4

....

! Linear system solver for outer loop Outer: Linear System Solver = "Iterative" Outer: Linear System Iterative Method = GCR Outer: Linear System GCR Restart = 250 Outer: Linear System Residual Output = 25 Outer: Linear System Max Iterations = 200 Outer: Linear System Abort Not Converged = False Outer: Linear System Convergence Tolerance = 1e-8

```
$blocktol = 0.001
block 11: Linear System Convergence Tolerance = $blocktol
block 11: Linear System Solver = "iterative"
block 11: Linear System Scaling = false
block 11: Linear System Preconditioning = ilu
block 11: Linear System Residual Output = 100
block 11: Linear System Max Iterations = 500
block 11: Linear System Iterative Method = idrs
```

block 22: Linear System Convergence Tolerance = \$blocktol

Advecting with the ice flow: ParticleAdvector

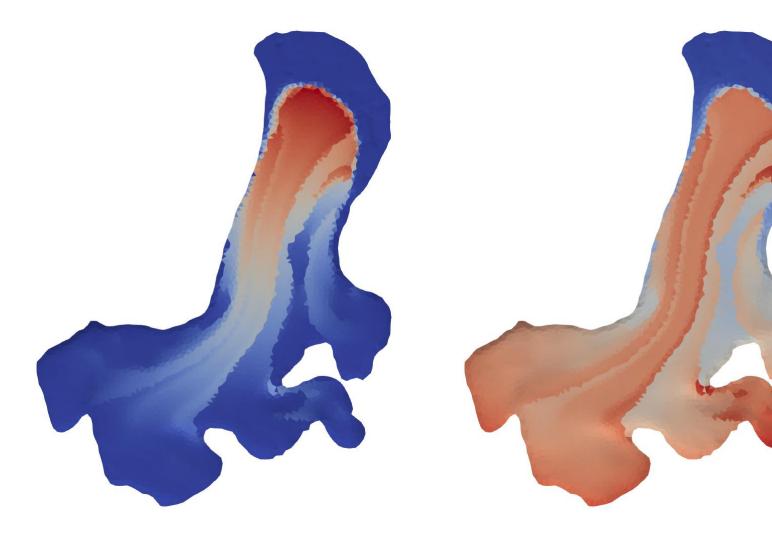
- Solver 5
- Uses ability to follow particles in the mesh

olnitially implemented for true physical particles

- Particles are made to travel backward in time along the flowlines
- Values may be integrated along the path or registered at the initial location

Equation = ParticleAdvector Procedure = "ParticleAdvector" "ParticleAdvector" ! Initialize particles at center of elements Advect Elemental = Logical True ! Timestepping strategy Particle Dt Constant = Logical False Max Timestep Intervals = Integer 1000 Timestep Unisotropic Courant Number = 0.25 Max Timestep Size = 1.0e3 Max Integration Time = Real 1.0e4 ! Integration forward in time Runge Kutta = Logical False Velocity Gradient Correction = Logical True Velocity Variable Name = String "Flow Solution" ! The internal variables for this solver Variable 1 = String "Particle Distance" Variable 2 = String "Particle Time Integral" ! The field variables being advected Variable 3 = String "Coordinate 1" Result Variable 3 = String "Advected Z" End





Distance travelled

Initial height of ice

Running the case



- In serial: ElmerSolver mlb.sif
- •In parallel, here with 4 processes: ElmerGrid 2 2 outline62_lc50 -partdual -metisrec 4 mpirun -np 4 ElmerSolver_mpi mlb.sif

•An my laptop the basic case takes

Things to test by yourself

- Running the initial case (cl₅0)
- Runnig the smaller/larger cases (cl75, cl25)
- Altering number of integration points • Does it have an affect on simulation results: ...,21, 28, 44, 64,...
- Trying effect of Courant number in particle advection
- ...
- You may turn off ParticleAdvector off if not needed as it uses a lot of time

 Exec Solver = never