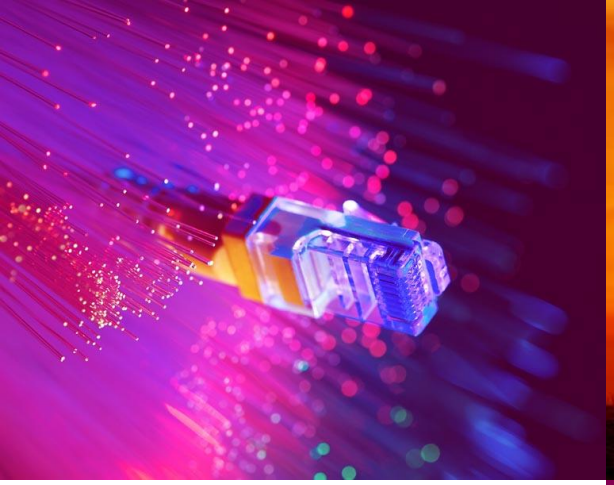


LUMI-Hackathon - Elmer

2024-09-26

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

ElmerSolver - Physical Models

- Heat transfer
  - ✓Heat equation
  - ✓Radiation with view factors
  - ✓convection and phase change
- Fluid mechanics
  - ✓ Navier-Stokes (2D & 3D)
  - ✓ RANS: *SST k-Ω, k-ε, v²-f*
  - ✓ LES: VMS
  - ✓ Thin films: Reynolds (1D & 2D)
- Structural mechanics
  - ✓ General elasticity (unisotropic, lin & nonlin, Maxwell)
  - ✓ Plates & Shells
- Acoustics
  - ✓ Helmholtz
  - ✓ Linearized time-harmonic N-S
  - ✓ Monolithic thermal N-S
- Species transport
  - ✓ Generic convection-diffusion equation
- Electromagnetics
  - ✓ Solvers for either scalar or vector potential (nodal elements)
  - ✓ Edge element based AV solver for magnetic and electric fields
- Mesh movement (Lagrangian)
  - ✓ Extending displacements in free surface problems
  - ✓ ALE formulation
- Level set method (Eulerian)
  - ✓ Free surface defined by a function
- Electrokinetics
  - ✓ Poisson-Boltzmann
- Thermoelectricity
- Quantum mechanics
  - ✓ DFT (Kohn Scham)
- Particle Tracker
- ....

Elmer in numbers

Software

- ~440,000 lines of active code
  - ~3/4 in Fortran, 1/4 in C/C++
- ~700 consistency tests
- ~800 pages of documentation
- ~1000 code commits yearly

Community

- ~20,000 downloads for Windows binary yearly
  - Linux users untracked
- ~2000 forum postings yearly
- ~100 people participate on Elmer courses yearly
- Several Elmer related scientifc visits to CSC yearly

Elmer and Elmer/Ice

- **Elmer** (= multi-physics package) with additional routines for Glaciology
- Maintained and supported by **CSC**
- **Open Source** (GPL2 or later)
  - Transparence (you co-own the code)
  - Sustainability (no license fees)
  - Viral effect of GPL (new code also GPL)
  - Linking to library allowed under LGPL
- Large international user community
  - Knowhow of well-established institutions
- Good level of support/documentation
  http://elmerice.elmerfem.org

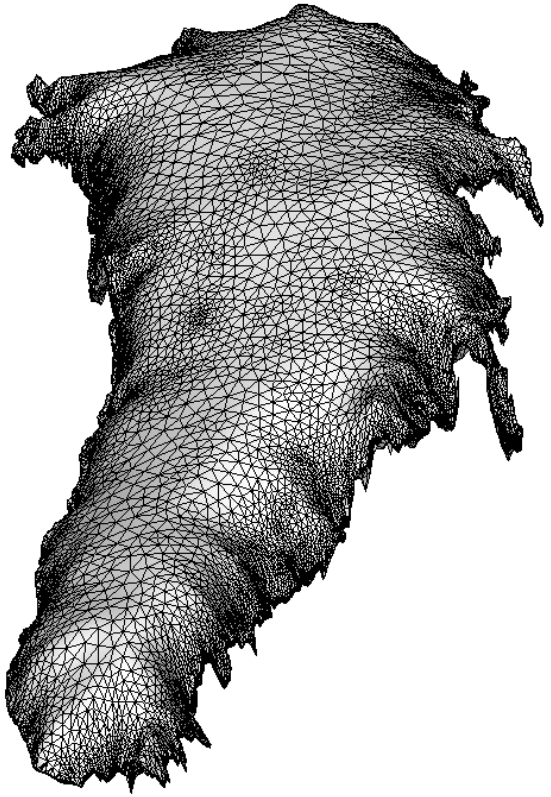
- Elmer/Ice builds on Elmer and includes developments related to glaciological problems. Elmer/Ice includes a variety of dedicated solvers and user functions for glaciological applications and their development is supported by various groups and funding…

norden
NordForsk

Tipping Points in Antarctic Climate Components

Elmer/Ice

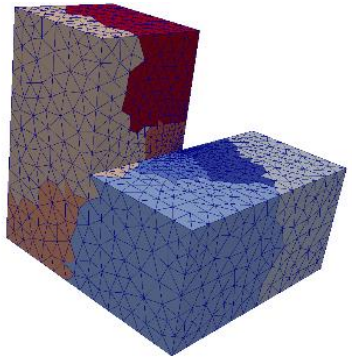
- **Full-Stokes** (also SIA and SSA) with post processing for stress/strain
- **Mesh:** Unstructured, vertically extruded, deforming and moving meshes
- **Temperature** solver accounting for pressure melting point or Enthalpy solver
- **Rheology:** Glen, anisotropy, firn densification, damage mechanics
- Special **sliding laws**: Weertman, Coulomb, Budd, Tsai
- Basal **hydrology** models (2): GlaDS and double continuum
- **NetCDF**-readers (for geometry as well as coupling to climate)
- Simple SMB (**PDD**)
- **Calving** models (3 approaches)
- **Inverse methods** for data assimilation
- Methods for **tracer transport/age-depth**



Getting Elmer ready for GPUs

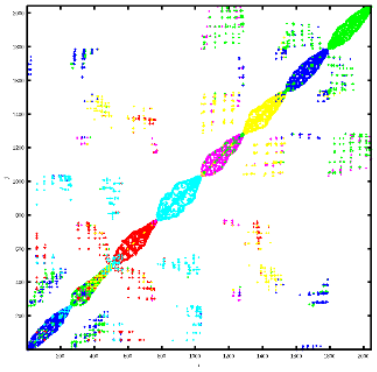
- **POP3 audit** with MPI + OMP SIMD CPU version (baseline for next audit using GPU offload)
- Working through **code**-base to reach **compatibility** with several involved compiler suites (gcc, clang, CrayCE) – LUMI needs Cray-Fortran to **enable OMP target** offloading!
- Working on different **interfaces for offloading linear system** solution step to GPUs (M250 and A100)

Elmer



MPI – domain decomposition

OpenMP



Target offload for **matrix assembly**

rocALUTION

AMD ROCm

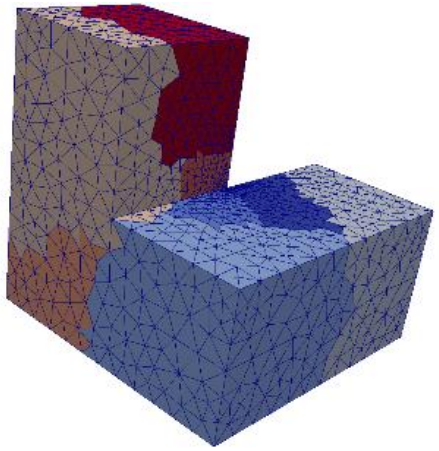
Sparse matrix solution library for particular GPU

Hackathon

- How many people involved from ELMER team?
  - 4 developers (J. Kataja, J. Ruokalainen, P. Råback, T. Zwinger) – underlined names present in Brussels
- Source code
  - https://github.com/ElmerCSC/elmerfem/tree/devel (source code, branch devel)
    - Should be ready to compile with Cray-CCE
    - External libraries needed: rocALUTION (incl. MPI !!), Hypre, MUMPS and eventually SuiteSparse

Hackathon

- What test case to work with?



- https://github.com/ElmerCSC/elmer-linsys/tree/cheese/Poisson/WinkelUnstructured-ChEESE
  - Was used to test on LUMI-C in **a CPU based POP3 audit**: https://co-design.pop-coe.eu/reports/POP3-AR-003-Elmer.html
  - Can run in a single node
  - Can also be easily scaled to span several nodes
  - Contains a **single solver** where we want to apply the **OpenMP target offload** directives
  - Runscripts for LUMI are included in the repository

Goals for Hackathon

- Profile and measure the current code and interpret the profiling results
  - Optimize accordingly
- Build a system so that user may provide material (c) and force (k) parameters
  - Precompute to nodes on CPU w/ ElmerLibrary
- Keep CSR matrix on GPU and call rocALUTION solvers
- Implement p-elements via reference element + linear map (might be too ambitious)

A more detailed and technical document for this Hackathon is to be found under
https://siili.rahtiapp.fi/omf2ouezQJSrAmVsjWIUcA?both#