



# Elmer on Intel Xeon Phi

# Elmer on Intel Xeon Phi

CSC-IT Center for Science Ltd.

Mikko Byckling ([mikko.byckling@csc.fi](mailto:mikko.byckling@csc.fi)),  
Olli-Pekka Lehto ([olli-pekka.lehto@csc.fi](mailto:olli-pekka.lehto@csc.fi)),  
Elmer Team

# Contents

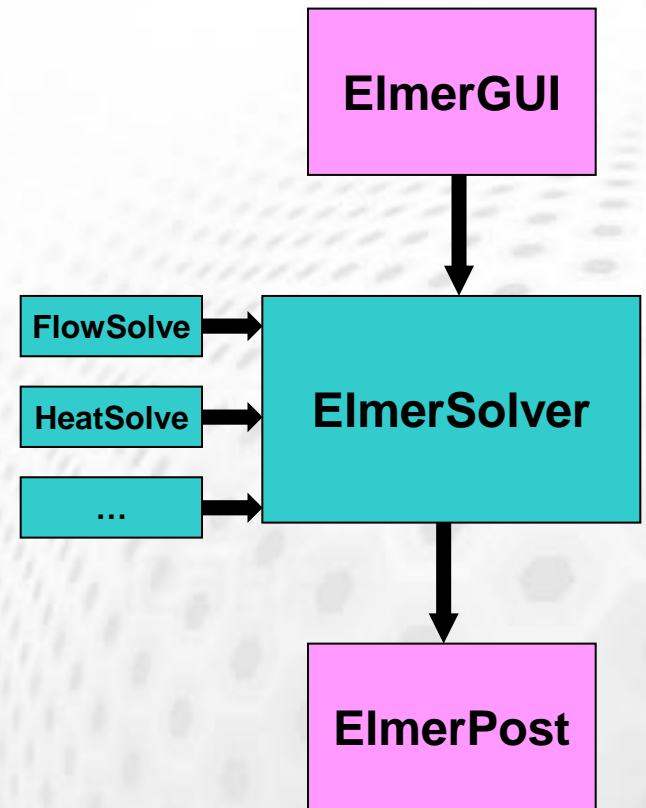
- Introduction to Elmer
- Porting Elmer to MIC
- Current status and performance
- Threading legacy code
- Future developments for Elmer
- Conclusions

# Elmer: Finite element software for multiphysical problems

- Developed and maintained by CSC
- Used by thousands of researchers worldwide
- Licensed under (L)GPLv2
- Contains a large set of ready-made physical models
- Readily extensible by end user
- <http://www.csc.fi/elmer>

# Elmer components

- Elmer is a suite of several programs
- Components can be used independently
- **ElmerGUI**: Pre- and Postprocessing
- **ElmerGrid**: structured meshing and mesh import
- **ElmerSolver**: Solution
- **ElmerPost**: Postprocessing
- **Others**: ElmerFront , ElmerParam, MATC, Mesh2D



## Elmer on Intel Xeon Phi (MIC)

- CPU: Preprocessing and mesh generation
- CPU/MIC: Solution of the physical problem
- CPU: Postprocessing of the results

### **Porting effort:**

ElmerSolver and associated libraries

# Elmer programming languages

- Fortran90 (and newer)
  - ElmerSolver (~210,000 lines, ~50% in DLLs)
- C++
  - ElmerGUI (~18,000 lines)
  - ElmerSolver (~10,000 lines)
- C
  - ElmerPost
  - ElmerGrid (~30,000 lines)
  - MATC (~11,000 lines)

# Elmer: Physical Models

## Heat transfer

- Heat equation
- Radiation with view factors
- convection and phase change

## Fluid mechanics

- Navier-Stokes (2D & 3D)
- RANS: SST  $k-\Omega$ ,  $k-\varepsilon$ ,  $v^2-f$
- LES: VMS
- Thin films: Reynolds (1D & 2D)

## Structural mechanics

- General Elasticity  
(anisotropic, lin & nonlin)
- Plate, Shell

## Acoustics

- Helmholtz
- Linearized time-harmonic N-S

## Species transport

- Generic convection-diffusion equation

## Electromagnetics

- Steady-state and harmonic analysis
- Whitney element formulation for magnetic fields

## Mesh movement (Lagrangian)

- Extending displacements in free surface problems
- ALE formulation
- Mortar finite elements

## Level set method (Eulerian)

- Free surface defined by a function

## Electrokinetics

- Poisson-Boltzmann

## Thermoelectricity

## Quantum mechanics

- DFT (Kohn Sham)

## Particle Tracker

...



# Elmer: Numerical Methods

- Time-dependency
  - Static, transient, eigenmode, scanning
- Discretization
  - Element families: nodal, edge, face, and p-elements, DG
  - Formulations: Galerkin, stabilization, bubbles
- Linear system solvers
  - Direct: Lapack, Umfpack, SuperLU, Mumps, Pardiso
  - Iterative Krylov subspace methods (Internal, Hypre)
  - Preconditioners: ILU, AINV, Multigrid (Internal, Hypre, Trilinos)
  - Multigrid solvers (GMG, AMG) (Internal, Hypre, Trilinos)
  - FETI (with Mumps)
- Parallellism (MPI / OpenMP)
  - Mesh multiplication, parallel finite element assembly
  - Linear system solution (Krylov methods, Multigrid)

## Elmer: Multiphysics features

- Solver is an abstract dynamically loaded object
  - May be developed and compiled using an API to the main library
  - No upper limit to the number of Solvers (currently ~50 available)
- Solvers may be active in different domains and meshes
  - Automatic mapping of field values
- Solvers may be weakly coupled without any *a priori* defined manner
- Tailored methods difficult strongly coupled problems
  - Consistent modification of equations (e.g. artificial compressibility in FSI, pull-in analysis)
  - Monolithic solvers (e.g. Linearized time-harmonic Navier-Stokes)

## Porting Elmer to MIC

- Porting work started Q2/12
- Focus to build ElmerSolver on a MIC
- Build process not entirely trivial
  - Initially tricks to fool automake
  - Manual editing of some resulting config-files
- ElmerSolver consistency tests
  - Initially 152 of 215 tests passed successfully
  - After a few hours of work 198 of 215 tests passed successfully

## Build process

- Elmer build process is based on automake
- Short term solution (current)
  - Trap `execve` to redirect configure test with `ssh`  
`LD_PRELOAD=./xmatic.so ./configure`
  - Manual editing of some Makefiles
- Long term solution(s) (in progress)
  - Using `binfmt_misc` from Linux kernel
  - Permanently switch to using `cmake`

## Automake with `binfmt_misc`

- Prequisites
  - Passwordless `ssh` access to MIC
  - Home directories mounted with `nfs`
- Set up `micrun` -script (`ssh` wrapper)
- Add K10M architecture definition to `binfmt_misc` dictionary to execute native MIC binaries via `micrun`
- Any application using automake can be cross-compiled to MIC with this approach

## Elmer OpenMP status

- ElmerSolver library routines are generally thread safe
- Environment variable **OMP\_NUM\_THREADS** must be set, the default is to use a single thread
- ElmerSolver internal tests run with **OMP\_NUM\_THREADS>1**
  - 228 of 231 tests pass successfully
  - Test failures are due to lack of tolerances

## Elmer OpenMP status (cont.)

### With `OMP_NUM_THREADS` undefined

```
> unset OMP_NUM_THREADS
> mpirun -np 2 ElmerSolver_mpi
ELMER SOLVER (v 7.0) STARTED AT: 2013/04/02 15:46:43
ELMER SOLVER (v 7.0) STARTED AT: 2013/04/02 15:46:43
ParCommInit: Initialize #PEs:          2
WARNING:: MAIN: OMP_NUM_THREADS not set. Using only 1 thread.
WARNING:: MAIN: OMP_NUM_THREADS not set. Using only 1 thread.
MAIN:
MAIN: =====
MAIN: ElmerSolver finite element software, Welcome!
MAIN: This program is free software licensed under (L)GPL
MAIN: Copyright 1st April 1995 - , CSC - IT Center for Science Ltd.
MAIN: Webpage http://www.csc.fi/elmer, Email elmeradm@csc.fi
MAIN: Library version: 7.0 (Rev: 6103M)
MAIN: Running in parallel using 2 tasks.
```

## Elmer OpenMP status (cont.)

### With `OMP_NUM_THREADS=4`

```
> export OMP_NUM_THREADS=4
> mpirun -np 2 ElmerSolver_mpi
ELMER SOLVER (v 7.0) STARTED AT: 2013/04/02 15:57:54
ELMER SOLVER (v 7.0) STARTED AT: 2013/04/02 15:57:54
ParCommInit: Initialize #PEs:          2
MAIN:
MAIN: =====
MAIN: ElmerSolver finite element software, Welcome!
MAIN: This program is free software licensed under (L)GPL
MAIN: Copyright 1st April 1995 - , CSC - IT Center for Science Ltd.
MAIN: Webpage http://www.csc.fi/elmer, Email elmeradm@csc.fi
MAIN: Library version: 7.0 (Rev: 6103M)
MAIN: Running in parallel using 2 tasks.
MAIN: Running in parallel with 4 threads per task.
```



## Elmer OpenMP status (cont.)

- Internally OpenMP threading supported by
  - Solver API routines related to element assembly
  - Time integration routines
  - Sparse matrix vector products
  - Element assembly loop of some solvers (MagnetoDynamics2D, ShallowWaterNS, StatElecSolve, ThermoElectricSolver)
- Library support for OpenMP exists in
  - External BLAS routines
  - External LAPACK routines
  - Direct solvers such as Cholmod, SPQR and Pardiso

# Finite element assembly

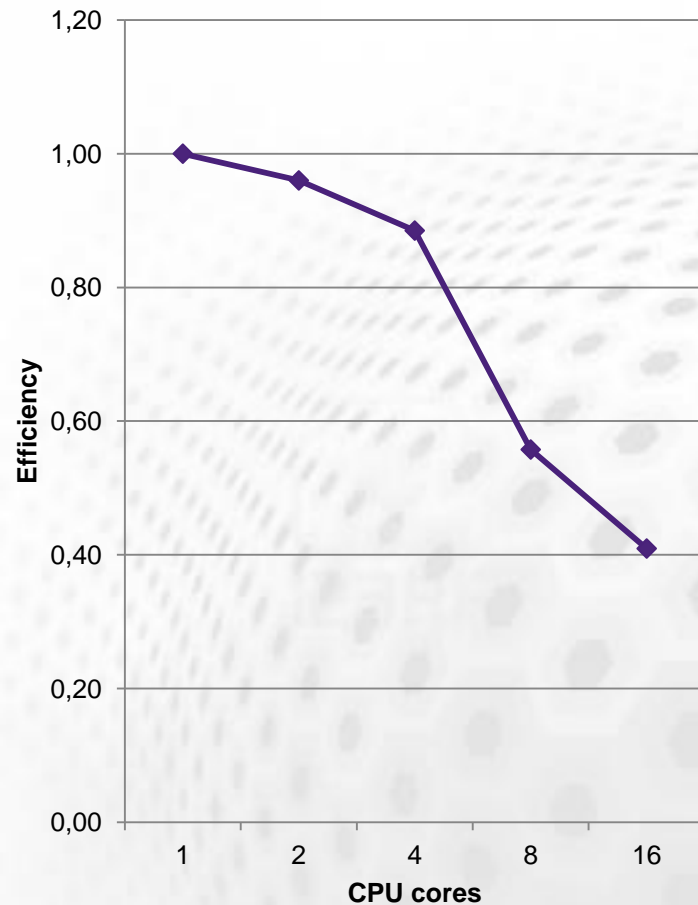
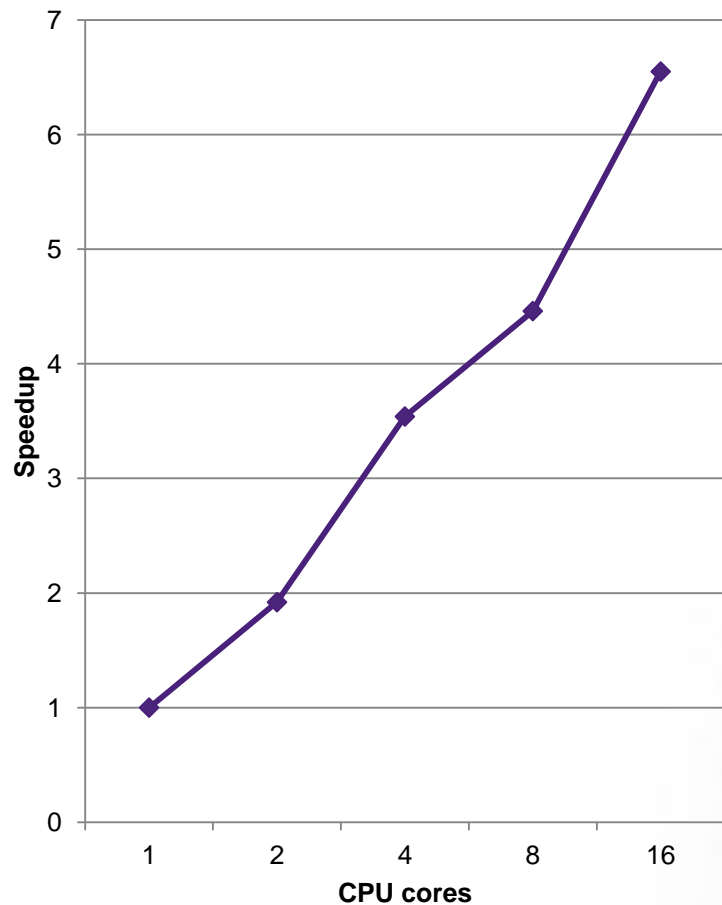
- Up to 20% of the runtime
- Linear workload growth with problem size
- Critical section needed in final step

Pseudocode:

```
for each Element in Elements in  
  parallel do  
    compute basis for Element  
    compute local matrix  
    glue local matrix to global matrix  
end do
```

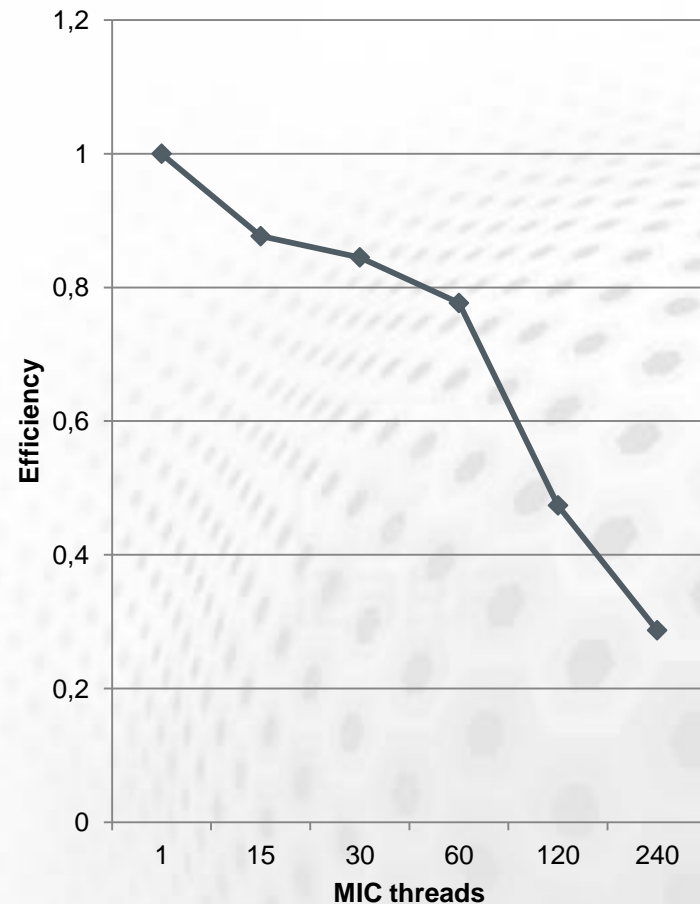
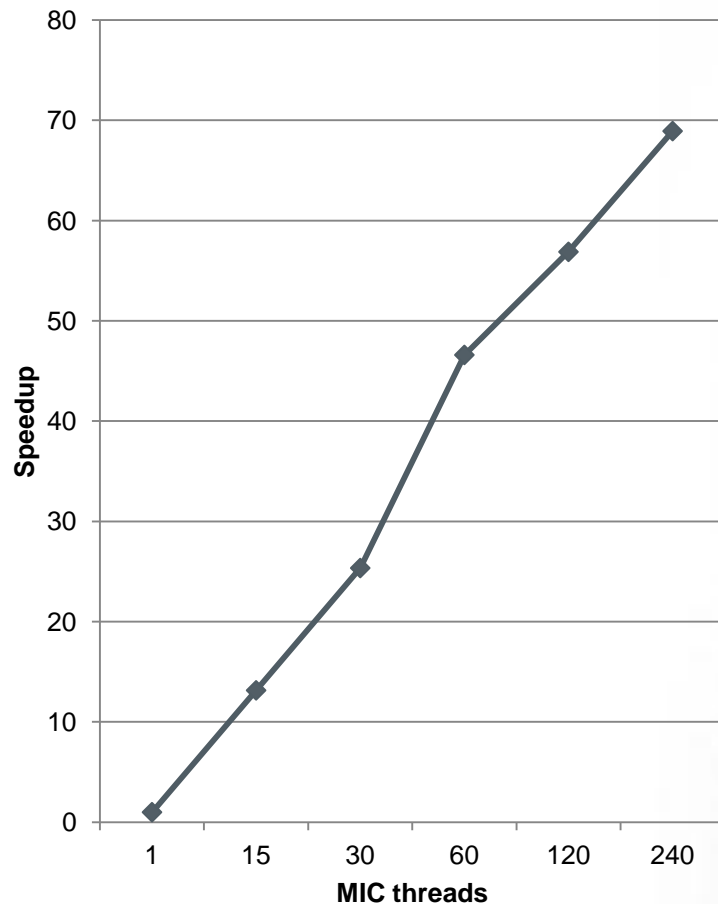
# Finite element assembly

Sandy Bridge E5, parallel scaling and efficiency



# Finite element assembly

Xeon Phi, parallel scaling and efficiency



# Sparse matrix-vector product, $y=Ax$

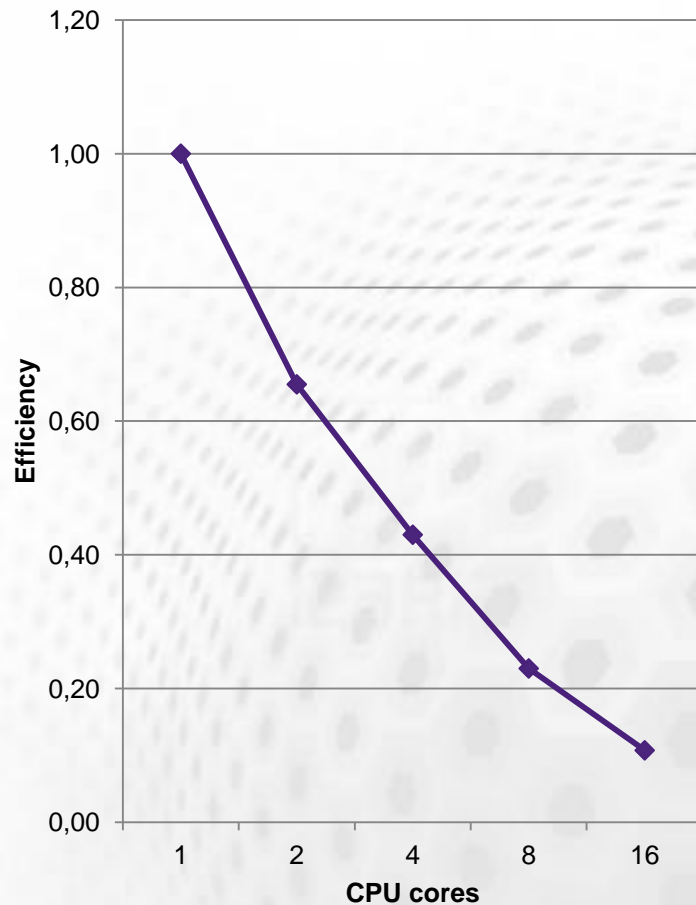
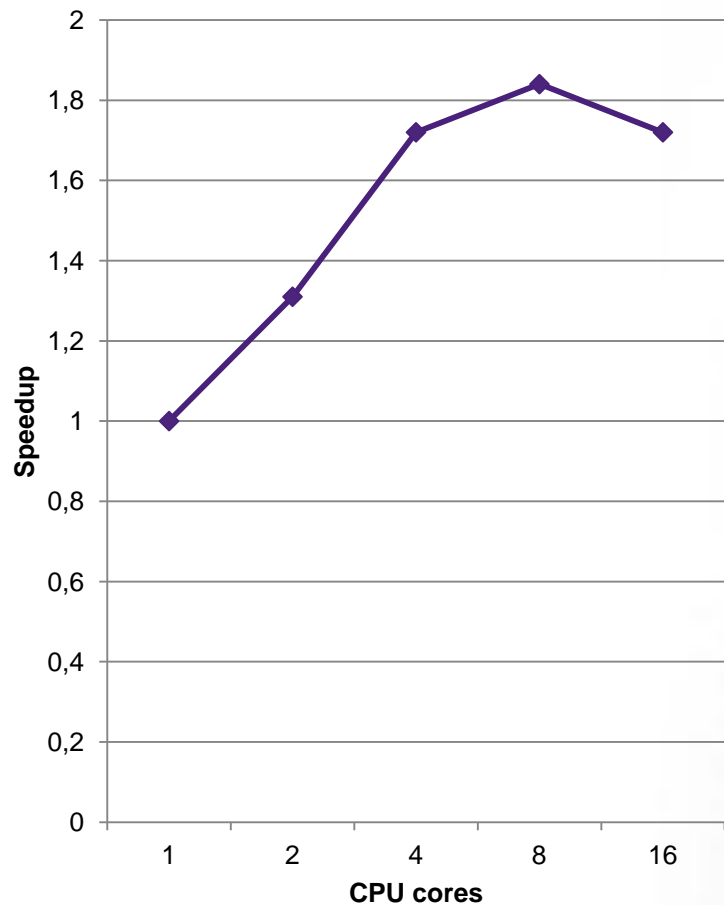
- Up to 80% of the total runtime
- Required by Krylov subspace methods
- Linear system solution is often the most challenging part as the model size increases

Pseudocode:

```
for i from 1 to n in parallel do  
  y(i)=0  
  for nonzero elements of A(i,:) do  
    y(i)=y(i)+A(i,j)*x(j)  
  end do  
end do
```

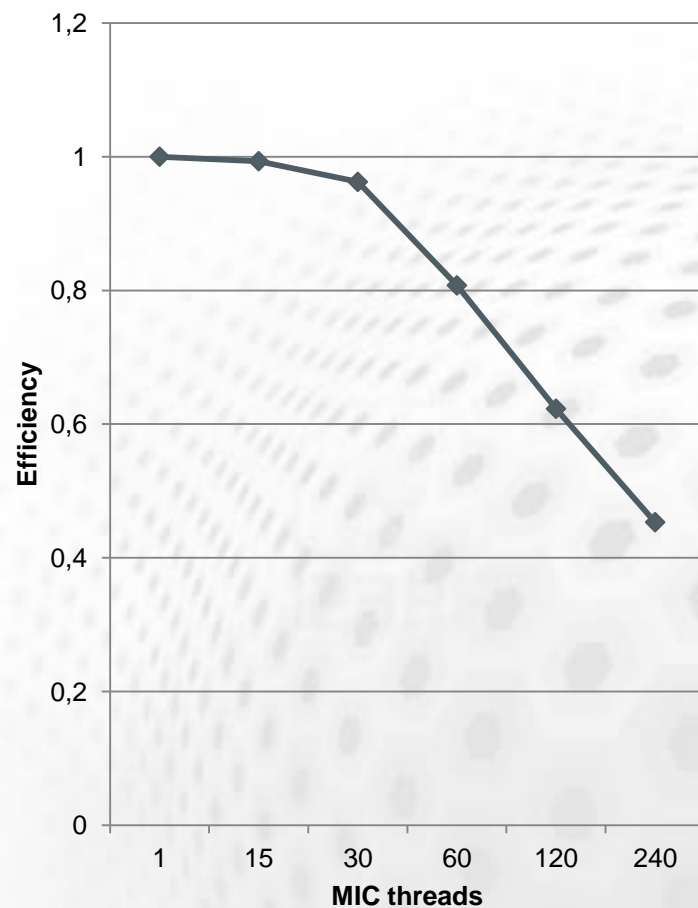
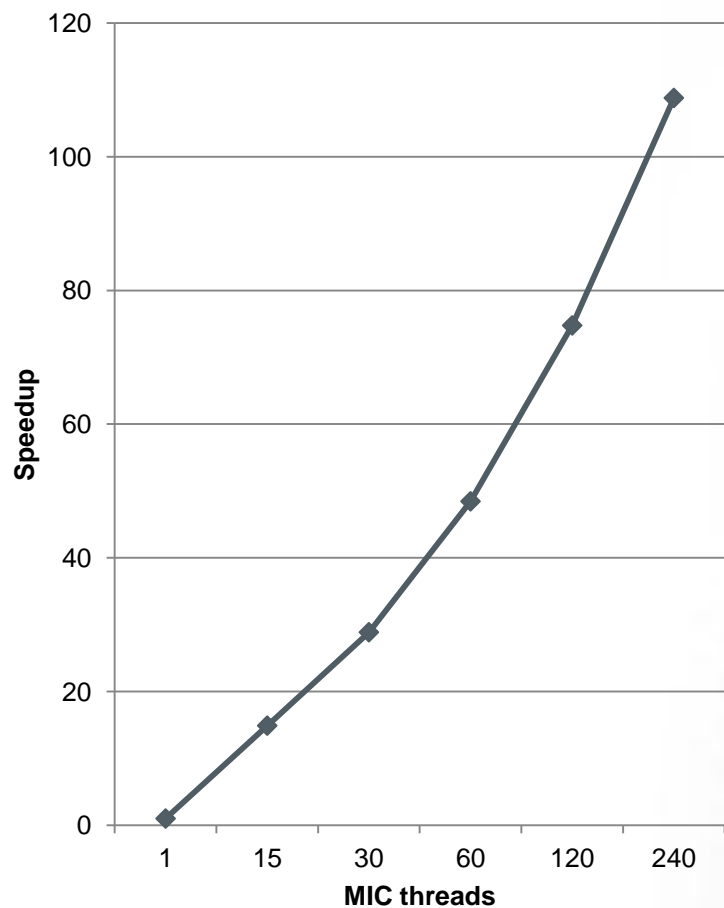
# SpDGEMv

Sandy Bridge E5, parallel scaling and efficiency



# SpDEGEMv

Xeon Phi, parallel scaling and efficiency



## Threading legacy code

- Single core performance of Xeon Phi is low => be aware of Amdahl's law
- Perform disruptive changes if necessary
- Use tools
  - Intel Inspector XE / Intel IDB (to find threading bugs)
  - Intel Vtune (to find hotspots)



## Future developments for Elmer

- Modify most important solvers to fully support OpenMP
- Modify ElmerSolver kernels to better support SIMD processing
- Expand ElmerSolver kernels to fully support OpenMP
- Experiment with offloading
- Implement parallel preconditioners

## Conclusions

- ElmerSolver libraries have been ported to Intel Xeon Phi
- Porting effort was relatively easy
- Performance optimizations are in development
- Added benefit: code improvements and optimizations will also benefit CPUs

# Elmer on Intel Xeon Phi

Thank you!  
Questions / Comments?