OpenMP threading and vectorization of MPI
Finite element code Elmer

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6th March 2018
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Elmer finite element software for multiphysical problems

Figures by Esko Järvinen, Mikko Lyly, Peter Råback, Timo Veijola (TKK) & Thomas Zwinger
Elmer codebase

► **Software**
  - ~600k lines of code, \( \frac{3}{4} \) Fortran and rest in C/C++
  - ~500 consistency tests
  - ~750 pages of documentation
  - ~1000 commits per year

► **Community**
  - ~20k downloads of Windows binary yearly
  - ~2k forum posts yearly
  - ~100 participants on Elmer courses yearly
  - Several Elmer related scientific visits on CSC yearly
The finite element method

1. Element loop
   1.1 Local matrix assembly
   1.2 Local to global glueing: gather/scatter store in a compressed sparse row (CSR) matrix structure

2. Solve the global linear system

1. Loop $K \in \mathcal{K}$
   1.1 $\hat{A}_{ij}^K = \int_K a(\phi_i, \phi_j) \, dx$
   1.2 $A_{\sigma_i^K, \sigma_j^K} = A_{\sigma_i^K, \sigma_j^K} + \hat{A}_{ij}^K$

2. $Ax = b$
Previously

Local matrix assembly (1.1 only)

- Optimizing *Elmer* finite element software on KNL – IXPUG annual Spring Conference 2017
  - Vectorization of high order basis function evaluations
  - Optimization of local matrix assembly
  - Comparison of HSW and KNL performance after and before optimizations

GEMM Assembly + vectorized basis functions
Glueing

CSR matrix is a triple

\[
\begin{align*}
(vals \in \mathbb{R}^{\text{NNZ}}, \text{rows} \in \mathbb{N}^{\text{rows}+1}, \text{cols} \in \mathbb{N}^{\text{NNZ}})
\end{align*}
\]

CSR add value algorithm in FEM: \((A_{\sigma_i^K,\sigma_j^K} = A_{\sigma_i^K,\sigma_j^K} + \hat{A}_{ij}^K)\)

1. Local to global index map: each local \(j\) corresponds to global index \(\sigma_j\).
2. Row value bounds:
   \[
   r_{\text{bottom}} = \text{rows}(\sigma_i) \ldots r_{\text{top}} = \text{rows}(\sigma_i + 1) - 1.
   \]
3. Value indices: Let \(c_{ij}\) be location of \(\sigma_j\) in \(\text{cols}(r_{\text{bottom}}:r_{\text{top}})\).
4. Add \(\hat{A}_{ij}\) to \(\text{vals}(c_{ij})\).

Optimizations:

3. Switch binary search to linear search.
4. Prefetch \(\text{vals}(c_{ij})\).
Parallelization of matrix assembly

The part “4. Add $\hat{A}_{ij}$ to $\text{vals}(c_{ij})$” is the only place for possible race conditions.

Possible solutions:

1. MPI: Partition mesh and assemble in serial in each rank.
   Avoids race conditions by construction.

2. Coloring
   - Color elements so that elements of certain color never meet.
   - Looping over elements of one color guarantees no race conditions.
   - Coloring can be done in threaded fashion.
   - No need for minimal coloring.

3. Concurrent access (\$omp atomic)
Krylov methods: Find solution from Krylov subspace

\[ \mathcal{K}_N = (b, Ab, A^2b, \ldots, A^N). \]

OpenMP

- Only one “interior” M-V product required for global product \( Ab \)
- Use mkl_dcsrgemv if MKL is available, otherwise use OpenMP pragmas:

```c
!$omp parallel do private(j,rsum)
DO i=1,n
   rsum = 0.0d0
!DIR$ IVDEP
   DO j=Rows(i),Rows(i+1)-1 ...
```
Test platforms

- HSW: 2 × 12 core Intel Haswell E5-2690v3 node.
- SKL: 2 × Intel® Xeon® Gold 6148, 2.4GHz, 20 cores/socket, 2 threads/core
- KNL: Colfax development platform with 7210 Intel Xeon Phi, at 1.3 GHz, 16GB of MCDRAM, 96GB DDR4 memory. Cache mode.

More details in appendices.
Assembly results on SKL

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OMP/MPI comparison on SKL

Multithreaded performance relative to pure MPI

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Results: model problem

- Poisson problem in unit cube, 64,000 hexas
  - 3rd order elements: 472,361 dofs
  - 5th order elements: 875,801 dofs
- Measure assembly and linear solve separately
  - Strong scalability on one node
- Parallelization scheme: MPI, OpenMP
Assembly: KNL vs HSW
Results: linear solve

- Fixed number (100) of BiCGSTab iterations
- Utilizing full node with OpenMP:
  \[ \frac{t(\text{KNL p2})}{t(\text{HSW p2})} \approx 0.5 \]
Challenges

- Elmer has been originally designed to be a pure MPI code
  - All $O(\#\text{Elements})$ algorithms without communication parallelize automatically with MPI

- Threading challenges
  - ILU(n) preconditioning
  - Disk IO
  - Construction of internal element data structures
  - CSR matrix formatting
Conclusion

▶ Threading critical path FEM:
  ▶ OpenMP assembly on par with MPI (optimally scaling) assembly
  ▶ Data layout of local assembly optimized for modern SIMD processors
  ▶ Krylov solvers parallelize easily with OpenMP pragmas
    ▶ CSR matrix vector product: call mkl_dcsrgemv
  ▶ Linear solve on KNL node faster than on HSW
    ▶ Memory bound algorithm: BiCGSTab
  ▶ Given recent developments Elmer is now a hybrid OpenMP-MPI code
    ▶ Threading controlled with environmental variables.

http://elmerfem.org https://github.com/ElmerCSC/elmerfem
Details (KNL and HSW)

- **KNL**:
  - Colfax development platform with 7210 Intel Xeon Phi, at 1.3 GHz, 16GB of MCDRAM, 96GB DDR4 memory.
  - Cache mode
  - Compile flags `-vecabi=cmdtarget -xMIC-AVX512 -align array64byte`

- **HSW**:
  - 2 × 12 core Intel Haswell E5-2690v3 node
  - 8 × 16 GB DDR4 memory at 2133 MHz
  - No hyperthreading
  - Compile flags `-xAVX -axCORE-AVX2,CORE-AVX-I -align array64byte -vecabi=cmdtarget`

- **Software stack**:
  - Intel Fortran 17.0.4 (20170411)
  - IntelMPI 17 update 3 build 20170405
  - MKL 20170003

- **Environment variables**:
  - `OMP_PROC_BIND=TRUE`
  - `I_MPI_FABRICS`: default (shm intranode)
Details (SKL)

- Intel® Xeon® Gold 6148, Dual socket server, 2.4GHz, 20 cores/socket, 40 cores, 80 threads
- Intel® Hyper-Threading Technology enabled
- Intel® Turbo Boost Technology enabled
- DDR4 192 GB, 2666 MHz
- RHEL* 7.3
- Intel® Composer 2017U4
- nr_hugepages=8000
- KMP_AFFINITY=scatter,granularity=fine
  I_MPI_FABRICS=shm:tmi
  I_MPI_PIN_PROCESSOR_LIST=allcores:map=bunch