Total efficiency of core components in Finite Element frameworks

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motivation

**today’s HPC facilities**

- comprise heterogeneous compute nodes
  - multicore CPU(s) + some accelerator very common (GPU, Cell)
  - next generation accelerators upcoming (Intel XEON Phi)
  - even heterogeneity on-a-chip (SoCs)
- cost efficiency dominated by *energy-efficiency*

**today’s large-scale FEM codes**

- have to adapt to target hardware
  - heterogeneity and frameworking
  - parallelisation of applications (DD mostly)
  - parallelisation of core components (e.g. 'linear solver on GPU’)
  - optimisation with respect to many details (data-flow and SIMD mostly)
- can we have the same results with less energy? → TTS vs TES
total efficiency

(some) aspects of efficiency

- numerical efficiency
  - dominates asymptotic behaviour and wall clock time
- hardware-efficiency
  - exploit all levels of parallelism provided by hardware (SIMD, multi-threading on a chip/device/socket, multi-processing in a cluster, hybrids)
  - then try to reach good scalability (communication optimisations, block comm/comp)
- energy-efficiency
  - by hardware mostly but codes may have to be adjusted (→ portability)

Hardware-oriented Numerics: Enhance both hardware- and numerical efficiency simultaneously, use (most) energy-efficient hardware where available! Attention: codependencies!

Today’s major example: (local) unstructured grid geometric Multigrid with Approximate Inverse smoothers on GPUs
Today’s (first) example: ingredients

- (local) geometric multigrid
- for unstructured grids
- with Approximate Inverse smoothers
- with FE transfer operators
- with clever DOF sorting
- on GPUs (and multicore CPUs)
- all based on one kernel: SpMV

why local?

- because large scale HPC starts ’in the little’ → on one heterogeneous compute node
- consider a very slow compute node → perfect scaling, but good?
- consider a very bad single-node implementation → perfect scaling, but good?
FE-gMG as a core-component

**Coarse grained parallelism by domain decomposition (Schwarz)**

1. use conformal coarse mesh as starting point
2. cluster patches for local problem assembly (structured and unstructured! - many HPC/GPGPU examples are structured)
3. load-balance patches
linear solver

**ScaRC pattern**

- define data-parallel solver pattern globally (multigrid)
- use special smoother as local solver: *recursion or blockwise local solver* $\rightarrow$ *FE-gMG*
- patch type determines solver components
- apply the smoother: global defect $\rightarrow$ local solvers (recursion or FE-gMG) $\rightarrow$ global correction

ScaRC-preconditioner:

1. $d \leftarrow b - Ax$
2. $y \leftarrow \sum_i R_i^T \text{MG}(d)$, where $\text{MG}(d)$:
   1. $d_i \leftarrow R_i d$
   2. $y_i \leftarrow \text{FE-gMG}(B_i, d_i)$
   3. $y \leftarrow \sum_i R_i^T y_i$
3. $x \leftarrow x + y$
FE-gMG

**concentrate all tuning in one kernel: sparse matrix vector multiply (SpMV)**
- in coarse-grid solver: preconditioned Krylov subspace methods
- smoother:
  - preconditioned Richardson iteration or
  - Krylov subspace method
  - local preconditioners by *approximate inverses*
- defect

**the remainings**
- a little BLAS-1 (dot-product, norm, scale, ...)
- important: *grid transfer operators* → can also be realised as SpMV

**advantages**
- flexibility (only matrices are switched) → blackbox
- oblivious of FE-space, dimension, ...
- performance-tuning concentrated

**disadvantages**
- we somewhat move the problem from solver to assembly of matrices
SpMV: CSR vs. ELLPACK-R

**SpMV kernel - performance**

- example: stiffness-matrices from a 3D-Poisson problem, left: $Q_1$, right $Q_2$ (more nonzeros)
- DOF numbering scheme: bright to dark $\rightarrow$ larger matrix-bandwidth

$\rightarrow$ porting CSR-SpMV to GPUs catastrophic (access pattern)
$\rightarrow$ numbering of DOFs / number of nonzeros performance-critical
SpMV on GPUs

**ELLPACK-R**

- store sparse matrix $S$ in two arrays $A$ (non-zeros in column-major order) and $j$ (column-Index for each entry in $A$)
- $A$ has $(\#\text{rows in } S) \times (\text{maximum } \#\text{non-zeros in rows of } S)$
- shorter rows are filled
- additional array $r1$ to store effective non-zeros count per row (get stop on row right)

\[
S = \begin{bmatrix}
    1 & 7 & 0 & 0 \\
    0 & 2 & 8 & 0 \\
    5 & 0 & 3 & 9 \\
    0 & 6 & 0 & 4
\end{bmatrix}
\Rightarrow
A = \begin{bmatrix}
    1 & 7 & * \\
    2 & 8 & * \\
    5 & 3 & 9 \\
    6 & 4 & *
\end{bmatrix}
\quad
j = \begin{bmatrix}
    0 & 1 & * \\
    1 & 2 & * \\
    0 & 2 & 3 \\
    1 & 3 & *
\end{bmatrix}
\quad
r1 = \begin{bmatrix}
    2 \\
    2 \\
    3 \\
    2
\end{bmatrix}
\]

**advantages**

- complete regular access pattern to $y$ and $A$
- GPU implementation:
  - one thread for each element $y_i$
  - access to all ELLPACK-R arrays and $y$ completely coalesced (column-major)
  - access on $x$: use texture-cache (FERMI: L2-cache)
  - no synchronisation between threads needed
  - no branch-divergence
  - in addition: multiple threads can access one row (ELLPACK-T)

*access to $x$ depends on non-zero pattern of $A$* $\rightarrow$ bandwidth given by DOF-numbering
smoother, coarse grid solver

- preconditioned Richardson iteration:
  \[
  x^{k+1} \leftarrow x^k + \omega M (b - Ax^k)
  \]

- CG or BiCGStab: preconditioner, defect, ...

smoother construction

- Jacobi only does not suffice
- good preconditioners often are inherently sequential
- preconditioner of the smoother reduced to SpMV
- \( \rightarrow \) Sparse Approximate Inverse
smoother construction

\textbf{SPAI}

\[ \| I - MA \|_F^2 = \sum_{k=1}^{n} \| e_k^T - m_k^T A \|_2^2 = \sum_{k=1}^{n} \| A^T m_k - e_k \|_2^2 \]

where \( e_k \) is the \( k \)-th unit vector and \( m_k \) the \( k \)-th row of \( M \). \( \rightarrow \) for \( n \) columns of \( M \rightarrow n \) least squares opt-problems:

\[ \min_{m_k} \| A^T m_k - e_k \|_2, \; k = 1, \ldots, n. \]

- use non-zero pattern of the stiffness matrix for \( M \)

\textbf{SAINV}

- \textit{Stabilised Approximate Inverse}
- calculate factorisation \( A^{-1} = Z D^{-1} Z^T \) where \( Z \) and \( D \) are calculated explicitly: \( A \)-biconjugation applied to unit base
- \( Z \) is assembled incompletely: use drop-tolerance
- no structure constraints possible (as opposed to SPAI)
- \( \rightarrow \) sometimes: better approximation of \( A^{-1} \)
- SAINV approximately as good as ILU(0)
- problem: inherently sequential
SpMV in gMG (2)

**SpMV in grid transfer:**
- two conformal FE-spaces $V_{2h}$ and $V_h$
- with Lagrange-Basis: interpolation (grid-transfer) can be expressed as SpMV

**prolongation matrix**

$$(P^h_{2h})_{i,j} = \varphi^{(j)}_{2h}(\xi^{(i)}_{h})$$

**restriction matrix**

$$R^h_{2h} = (P^h_{2h})^T$$

- DOF numbering technique $\rightarrow$ performance
results

benchmark

- popular grid, unstructured, Poisson problem
- 2D and 3D, $Q_1$ and $Q_2$ FE, CPU (Core i7 980X, 6 threads) and GPU (Tesla C2070)
- Approximate Inverse strong smoothing (SPAI, SAINV)

\[
\begin{align*}
-\Delta u &= 1, \quad x \in \Omega \\
u &= 0, \quad x \in \Gamma_1 \\
u &= 1, \quad x \in \Gamma_2
\end{align*}
\]

- different FE-spaces
- different DOF numbering techniques
## FE-gMG: (2D)

|        | CPU |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |
|--------|-----|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
|        |     | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   |
|        | sort| time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  |
| 2lv    |     | 4.04     | 13       | 2.54     | 5        | 1.59     | 3.59     | 6        | 1.12     | 1.06     | 13       | 3.82     | 0.56     | 5        | 1.88     | 4.53     | 0.56     | 5        | 1.88     | 4.53     | 1.19     | 6        | 0.89     | 3.01     | 1.19     | 6        | 0.89     | 3.01     |
| CM     |     | 3.65     | 13       | 2.19     | 5        | 1.66     | 3.29     | 6        | 1.11     | 1.03     | 13       | 3.55     | 0.72     | 5        | 1.43     | 3.05     | 0.82     | 6        | 1.26     | 4.03     |          |          |          |          |          |          |          |          |
| XYZ    |     | 3.48     | 13       | 2.06     | 5        | 1.69     | 4.44     | 9        | 0.78     | 0.98     | 13       | 3.53     | 0.51     | 5        | 1.93     | 4.04     | 1.03     | 9        | 0.96     | 4.32     |          |          |          |          |          |          |          |          |          |
| Stoch  |     | 4.04     | 13       | 2.57     | 5        | 1.57     | 3.19     | 5        | 1.27     | 1.74     | 13       | 2.33     | 1.04     | 5        | 1.66     | 2.46     | 1.29     | 5        | 1.35     | 2.47     |          |          |          |          |          |          |          |          |          |
| Hie    |     | 3.49     | 13       | 2.07     | 5        | 1.69     | 3.07     | 6        | 1.14     | 0.97     | 13       | 3.59     | 0.50     | 5        | 1.94     | 4.14     | 0.77     | 6        | 1.26     | 3.98     |          |          |          |          |          |          |          |          |          |

## FE-gMG: (3D)

|        | CPU |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |          |
|--------|-----|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|----------|
|        |     | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   | SPAI     | SAINV    | Jacobi   |
|        | sort| time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  | time     | #iter    | speedup  |
| 2lv    |     | 2.43     | 26       | 1.08     | 7        | 2.25     | 1.03     | 9        | 2.37     | 0.66     | 26       | 3.71     | 0.27     | 7        | 2.39     | 3.94     | 0.28     | 9        | 2.32     | 3.63     |          |          |          |          |          |          |          |          |          |
| CM     |     | 2.34     | 26       | 1.02     | 7        | 2.30     | 0.98     | 9        | 2.37     | 0.66     | 26       | 3.53     | 0.28     | 7        | 2.39     | 3.67     | 0.29     | 9        | 2.26     | 3.36     |          |          |          |          |          |          |          |          |          |
| Stoch  |     | 2.63     | 26       | 1.18     | 7        | 2.23     | 1.28     | 10       | 2.06     | 0.75     | 26       | 3.48     | 0.33     | 7        | 2.32     | 3.61     | 0.38     | 10       | 1.98     | 3.35     |          |          |          |          |          |          |          |          |          |

## Results

- **Jacobi**: Sequentially calculated.
- **SPAI**: Preconditioned by SPAI.
- **SAINV**: Preconditioned by SAINV.
FE-gMG: combined effects: gMG + AI smoother + DOF numbering + GPU
results

**complete geometric multigrid on GPUs**

- completely unstructured grids possible
- high extensibility potentials: smoother
- DOF-numbering still critical
- careful combination of hardware- and numerical efficiency offers up to 3 orders of magnitude speedup!
- matrix assembly not considered (stiffness/mass, transfer, preconditioner) → random access matrices needed!
heterogeneity on a node also means incorporating all resources!

**example solver: SWE with multiple extensions**

- hardware-oriented numerics: use well parallelisable algorithms, where possible (accuracy!)
- here: sophisticated free-surface flow solver based on SWE solved with LBM (bed friction, wind, pollutant transport, FSI): MPI + PThreads + SSE + CUDA

\[
\begin{align*}
\frac{\partial h}{\partial t} + \frac{\partial (hu_j)}{\partial x_j} &= 0 \quad \text{and} \quad \frac{\partial h u_i}{\partial t} + \frac{\partial (h u_i u_j)}{\partial x_j} + g \frac{\partial}{\partial x_i} \left( \frac{h^2}{2} \right) = S_{i}^{\text{bed}} + S_{i}^{\text{wind}} \\
\frac{\partial h c}{\partial t} + \frac{\partial (hu_j c)}{\partial x_j} &= \frac{\partial}{\partial x_j} \left( Dh \frac{\partial c}{\partial x_j} \right) + S_{i}^{\text{poll}} \\
S_{i}^{\text{bed}} &= -g \left( h \frac{\partial b}{\partial x_i} + n_b^2 h^{-\frac{1}{3}} u_i \sqrt{u_j u_j} \right) \\
S_{i}^{\text{wind}} &= (\rho_\alpha 10^{-3} \times (0.75 + 0.0067 \sqrt{w_1^2 + w_2^2}))(w_1 \sqrt{w_1^2 + w_2^2}) \\
S_{i}^{\text{poll}} &= -Khc + S_0 h
\end{align*}
\]
heterogeneity on a node also means incorporating all resources!

**LBM for SWE**

\[ f_\alpha(x + e_\alpha \Delta t, t + \Delta t) = f_\alpha(x, t) + Q(f_\alpha, f_\beta), \quad \beta = 1, \ldots, k. \]

\[ f_\alpha^{\text{temp}}(x, t) = f_\alpha(x, t) - \frac{1}{\tau}(f_\alpha - f_\alpha^{\text{eq}}) \]

\[ f_\alpha^{\text{eq}} = \begin{cases} h(1 - \frac{5g}{6e^2} - \frac{2}{3e^2} u_i u_i) & \alpha = 0 \\ h(\frac{gh}{6e^2} + \frac{e_\alpha u_i u_i}{3e^2} + \frac{e_\alpha j u_i u_j}{6e^2} - \frac{u_i u_j}{8e^2}) & \alpha = 1, 3, 5, 7 \\ h(\frac{gh}{24e^2} + \frac{e_\alpha u_i u_i}{12e^2} + \frac{e_\alpha j u_i u_j}{12e^2} - \frac{u_i u_j}{24e^2}) & \alpha = 2, 4, 6, 8 \end{cases} \]

\[ f_\alpha(x + e_\alpha \Delta t, t + \Delta t) = f_\alpha(x, t) - \frac{1}{\tau}(f_\alpha - f_\alpha^{\text{eq}}) + \frac{\Delta t}{6e^2} e_\alpha i S_i, \quad \alpha = 0, \ldots, 8. \]

\[ h(x, t) = \sum_\alpha f_\alpha(x, t) \quad \text{and} \quad u_i(x, t) = \frac{1}{h(x, t)} \sum_\alpha e_\alpha i f_\alpha, \]

\[ g_\alpha^{\text{temp}}(x, t) = g_\alpha(x, t) - \frac{1}{\tau_{\text{var}}}(g_\alpha - g_\alpha^{\text{eq}}) \]

\[ \tau_{\text{poll}} = 1/2 + h(x, t) \times (\tau_{\text{poll}} - 1/2) \]

\[ g_\alpha^{\text{eq}} = \begin{cases} c(h - 5/9) & \alpha = 0 \\ c(1/9 + \frac{h}{3e^2} e_\alpha i u_i) & \alpha = 1, 3, 5, 7 \\ c(1/36 + \frac{h}{12e^2} e_\alpha i u_i) & \alpha = 2, 4, 6, 8 \end{cases} \]
heterogeneity on a node also means incorporating all resources!

example, single node performance

- CINECA IBM-PLX GPU cluster:
  - 2 6-core Westmeres and 2 NVIDIA Tesla GPUs per node
  - Infiniband
  - full features (flow + pollutant)
  - $2^l \times (2000 \times 2000)$ lattice sites and $3 \times 2^l$ nodes on refinement level $l$
heterogeneous compute nodes

eexample, scaling and finals

- optimisation concerning vectorisation is crucial for CPU performance
- in some cases: compiler unable to vectorise kernel loops at all (bed force term)
- good serial performance only granted by organising loops / register usage by hand
- hybrid pays off (10 percent is quite good!), if CPU kernels are reasonably optimised, load reasonably balanced
total time to solution vs total energy to solution

so far: combining hardware- and numerical efficiency

- now: what about energy?
- example: GPGPU: specialist accelerator
- in general: exploiting hardware that is considered to be more energy-efficient because it stems from the embedded fields (lower transistor count due to lower instr. set compatibility, mainly)
- often acceptable: decrease in total energy consumption bought with increase of total time to solution

example: TIBIDABO prototype cluster (BSC)

- 1 NVIDIA Tegra 2 SoC (dual core ARM Cortex-A9) per core
- LPDDR2 memory at low timings
- no SIMD
ARM vs x86

**TIBIDABO vs LiDO**
- TIBIDABO ARM cluster, up to 96 nodes
- Dortmund x86 cluster LiDO, up to 32 nodes (2x Nehalem dual socket quad core, SSE, DDR3)
conclusions

total efficiency

- hardware efficiency and numerical efficiency have to be augmented carefully and simultaneously → codependencies
- less total time to solution can (quite) easily be traded for less energy consumption
- energy efficiency of ARM architecture is (and is expected to be) increasing rapidly (SIMD, better caches, faster memory)

TODOs

- matrix assembly!!
- ’block-Jacobi’ character of the parallel scheme
- overlapping comm/comp
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