Performance Evaluation of Acoustic Material Implementation in SeisSol Using Roofline Model

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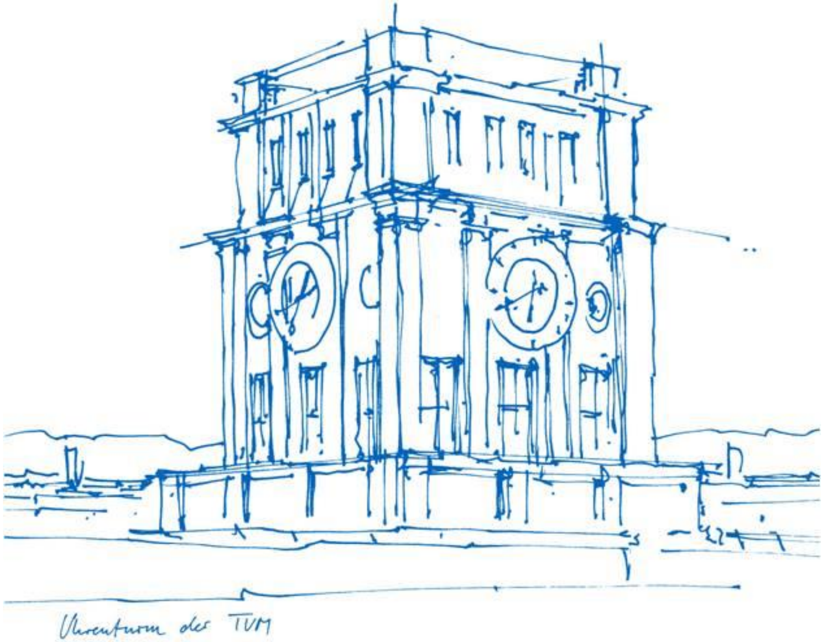


Content

- Physical Models
- Roofline Model
- Experimental Analysis
- Conclusion and Future Work

SeisSol

An open-source software for the simulation of seismic wave phenomena and earthquake dynamics

- Arbitrary high-order DERivative Discontinuous Galerkin method (ADER-DG)
  - ADER temporal discretization
  - DG spatial discretization

- Models of medium materials for seismic wave propagation
  - Elastic: isotropic and anisotropic
  - Poroelastic
  - Viscoelastic
  - Off-fault plastic
  - ...
  - How about acoustic? Water, air, oil?

  The ocean covers approximately 70% of Earth's surface!

Elastic Wave Model

Consider an infinitesimal cube near any point within a material:

Symmetric strain matrix: $\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{pmatrix}$, symmetric stress matrix: $\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix}$

The generalized Hooke's law relates stress and strain (under small perturbation assumption):

$\sigma_{ij} = \lambda\delta_{ij}\sum_{k=1}^{3}\varepsilon_{kk} + 2\mu\varepsilon_{ij}$, derivative with respect to time: $\frac{\partial\sigma_{ij}}{\partial t} = \lambda\delta_{ij}\sum_{k=1}^{3}\frac{\partial v_k}{\partial x_k} + \mu(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i})$

Newton's second law:

$\frac{\partial}{\partial t}\int_{\Omega}\rho\frac{\partial \boldsymbol{u}}{\partial t}\,dV = \int_{\partial\Omega}\boldsymbol{T}(\boldsymbol{n})\,dS + \int_{\Omega}\boldsymbol{f}\,dV$, differential form: $\rho\frac{\partial v_i}{\partial t} = \sum_{j=1}^{3}\frac{\partial\sigma_{ij}}{\partial x_j} + f_i$

Finally, $\frac{\partial \boldsymbol{q}}{\partial t} + \boldsymbol{A}(\boldsymbol{x})\frac{\partial \boldsymbol{q}}{\partial x_1} + \boldsymbol{B}(\boldsymbol{x})\frac{\partial \boldsymbol{q}}{\partial x_2} + \boldsymbol{C}(\boldsymbol{x})\frac{\partial \boldsymbol{q}}{\partial x_3} = 0$ with $\boldsymbol{q} = (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{23}, \sigma_{13}, v_1, v_2, v_3)^T$

$$\hat{\boldsymbol{A}}(\boldsymbol{x},\boldsymbol{n}) = n_1\boldsymbol{A}(\boldsymbol{x}) + n_2\boldsymbol{B}(\boldsymbol{x}) + n_3\boldsymbol{C}(\boldsymbol{x}) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -n_1(\lambda+2\mu) & -n_2\lambda & -n_3\lambda \\ 0 & 0 & 0 & 0 & 0 & 0 & -n_1\lambda & -n_2(\lambda+2\mu) & -n_3\lambda \\ 0 & 0 & 0 & 0 & 0 & 0 & -n_1\lambda & -n_2\lambda & -n_3(\lambda+2\mu) \\ 0 & 0 & 0 & 0 & 0 & 0 & -n_2\mu & -n_1\mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -n_3\mu & -n_2\mu \\ 0 & 0 & 0 & 0 & 0 & 0 & -n_3\mu & 0 & -n_1\mu \\ -\frac{n_1}{\rho} & 0 & 0 & -\frac{n_2}{\rho} & 0 & -\frac{n_3}{\rho} & 0 & 0 & 0 \\ 0 & -\frac{n_2}{\rho} & 0 & -\frac{n_1}{\rho} & -\frac{n_3}{\rho} & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{n_3}{\rho} & 0 & -\frac{n_2}{\rho} & -\frac{n_1}{\rho} & 0 & 0 & 0 \end{pmatrix}$$

(neglecting f_i)

Acoustic Wave Model

Hydrostatic model: $\frac{\partial p_0}{\partial x_1} = \frac{\partial p_0}{\partial x_2} = \frac{\partial p_0}{\partial t} = \frac{\partial \rho_0}{\partial x_1} = \frac{\partial \rho_0}{\partial x_2} = \frac{\partial \rho_0}{\partial t} = 0$, $\boldsymbol{v_0}(\boldsymbol{x}, t) = 0$

Small perturbation: $(\boldsymbol{v}(\boldsymbol{x}, t), \rho(\boldsymbol{x}, t), p(\boldsymbol{x}, t))^T = (\boldsymbol{v_0}(\boldsymbol{x}), \rho_0(\boldsymbol{x}), p_0(\boldsymbol{x}))^T + (\boldsymbol{v'}(\boldsymbol{x}, t), \rho'(\boldsymbol{x}, t), p'(\boldsymbol{x}, t))^T$

Mass conservation: $\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{v}) = 0$ -> $\frac{\partial p'}{\partial t} + K \sum_{k=1}^{3} \frac{\partial v'_k}{\partial x_k} - \rho_0 g v'_3 = 0$, bulk modulus: $K = \rho_0 \frac{dp}{d\rho}$

Momentum conservation: $\frac{\partial \rho \boldsymbol{v}}{\partial t} + \nabla \cdot (\boldsymbol{v} \otimes \rho \boldsymbol{v} + \boldsymbol{I} p) - \boldsymbol{f} = 0$ -> $\rho_0 \frac{\partial \boldsymbol{v'}}{\partial t} + \nabla \cdot (\boldsymbol{I} p') + \frac{\rho_0 g p'}{K} \boldsymbol{e_3} = 0$

Finally, neglecting the gravitational acceleration g :

$\frac{\partial \boldsymbol{q^{ac}}}{\partial t} + \boldsymbol{A^{ac}}(\boldsymbol{x}) \frac{\partial \boldsymbol{q^{ac}}}{\partial x_1} + \boldsymbol{B^{ac}}(\boldsymbol{x}) \frac{\partial \boldsymbol{q^{ac}}}{\partial x_2} + \boldsymbol{C^{ac}}(\boldsymbol{x}) \frac{\partial \boldsymbol{q^{ac}}}{\partial x_3} = 0$, with $\boldsymbol{q^{ac}} = (p', v'_1, v'_2, v'_3)^T$

$$\hat{\boldsymbol{A}}^{\boldsymbol{ac}}(\boldsymbol{x}, \boldsymbol{n}) = n_1 \boldsymbol{A^{ac}}(\boldsymbol{x}) + n_2 \boldsymbol{B^{ac}}(\boldsymbol{x}) + n_3 \boldsymbol{C^{ac}}(\boldsymbol{x}) = \begin{pmatrix} 0 & n_1 K & n_2 K & n_3 K \\ \frac{n_1}{\rho_0} & 0 & 0 & 0 \\ \frac{n_2}{\rho_0} & 0 & 0 & 0 \\ \frac{n_3}{\rho_0} & 0 & 0 & 0 \end{pmatrix}$$

Elastic vs Acoustic

When $\mu = 0$, the elastic model reduces to the acoustic model: $\boldsymbol{q} = (\sigma_{ii}, \sigma_{ii}, \sigma_{ii}, 0, 0, 0, v_1, v_2, v_3)^T$

Physical explanation of fluids: pressure is isotropic, no shear strain (stress)

Acoustic materials are a subset of elastic materials: $\sigma_{ii} = -p$

Current acoustic SeisSol: solving 9 PDEs for 4 DOFs (degrees of freedom)

But solving 4 PDEs are enough!

Kernels can be reused!

Performance comparison of elastic (with $\mu = 0$) and acoustic models

Target Application: SeisSol-Proxy

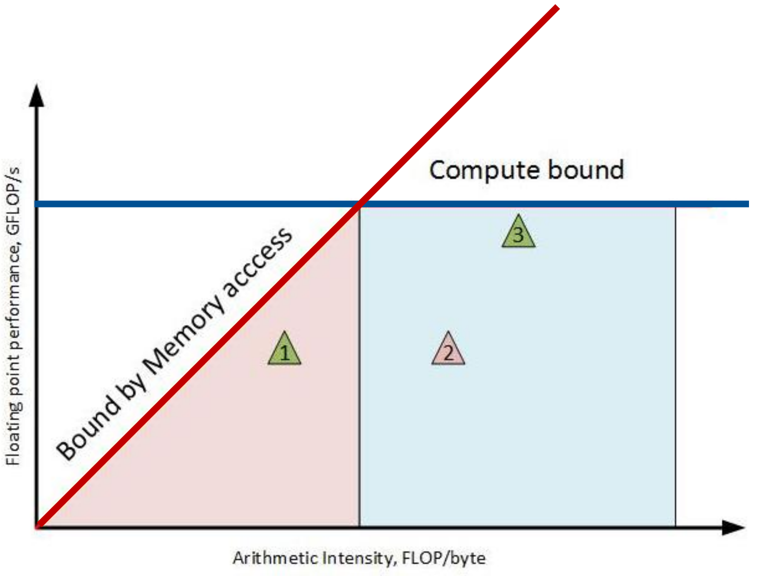
Proxy or mini applications are typically simple and lightweight but capture the core computational characteristics of the main simulation program.

- C++ OpenMP program run on a single node (all cores without SMT) of CoolMUC-2 at LRZ
- Parameters specified when building: physical model, accuracy order, host architecture (Haswell), numerical precision (double)
- $\mu = 0$ is hard-coded in the source code of the elastic model (only for SeisSol-proxy)
- `$ ./<proxy_executable> <num_cells> <num_timesteps> <kernel>`
  - `<kernel> = all` is executed `<num_timesteps> = 100` times on `<num_cells>` cells in parallel.
  - Iterations -> OpenMP threads: static scheduling
  - OpenMP threads -> hardware threads: one-to-one, pinned by LIKWID
  - First touch to avoid NUMA issue and load LLC for more accurate timing
  - Non-zero FLOP vs **hardware FLOP**

Roofline Model

A visual model used to analyze and optimize the performance of compute-intensive applications, which helps identify performance bottlenecks by comparing computational performance (FLOPS) with data throughput (memory bandwidth).

- Arithmetic (operational, computational) intensity:
  - Large value suggests compute-bound scenarios
  - Small value suggests memory-bound scenarios
- Components:
  - Peak performance (FLOPS)
  - Maximum data throughput (memory bandwidth)
  - Application points (arithmetic intensity, FLOPS)

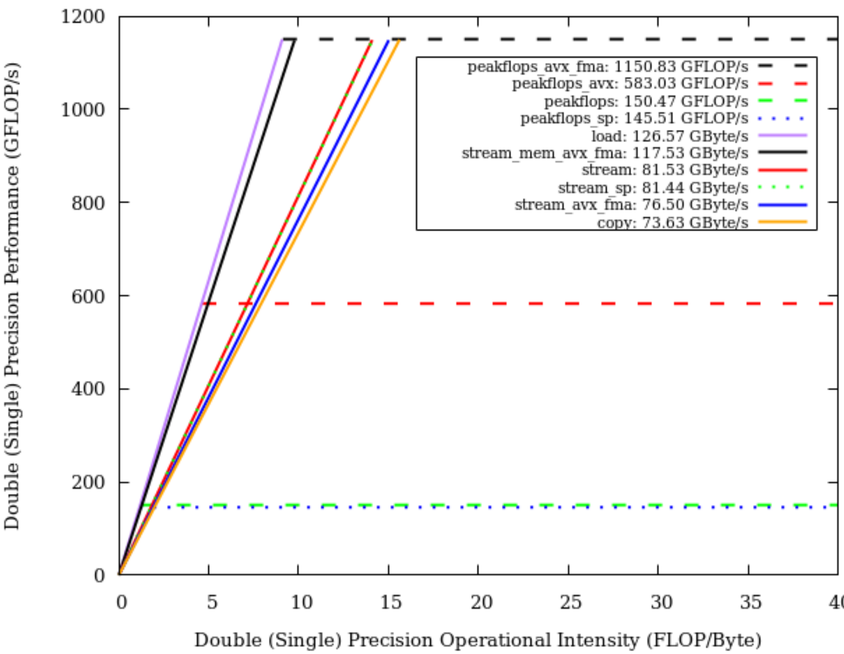


Roofline Models: Different Becnmarks

- Why benchmarks?
  - No full parallelization and vectorization
  - Ideal IPC
  - Thermal constraints

- Peak FLOPS
  - Precision
  - Vectorization
  - FMA

- Maximum memory bandwidth
  - `load (scalar=A[i])`
  - `copy (A[i]=B[i])`
  - `stream (A[i]=B[i]+scalar*C[i])`
  - `[_mem]`: non-temporal write

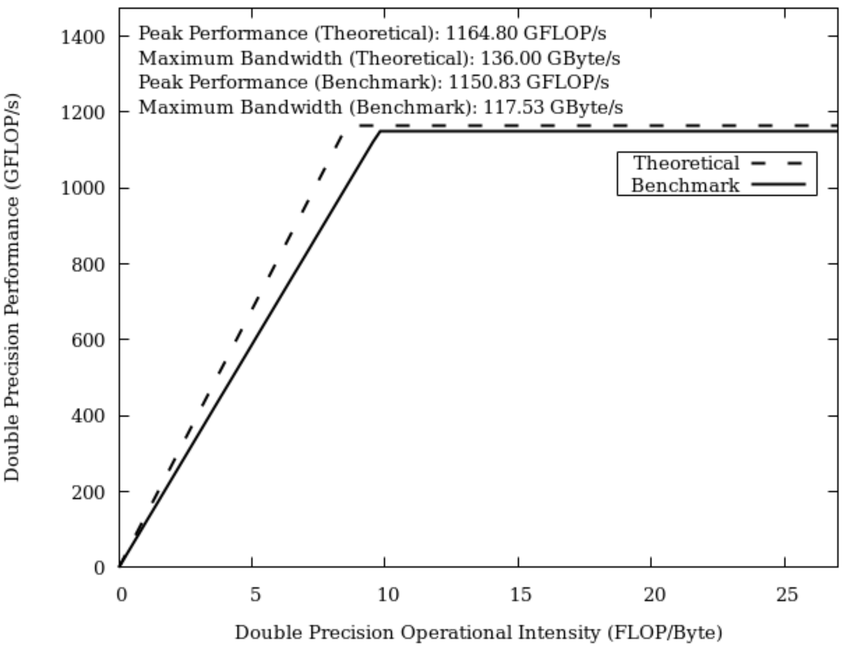


Roofline Models: Theoretical vs Benchmark

- Which benchmarks?
  - `peakflops_avx_fma`
  - `stream_mem_avx_fma` (read:write = 2:1)

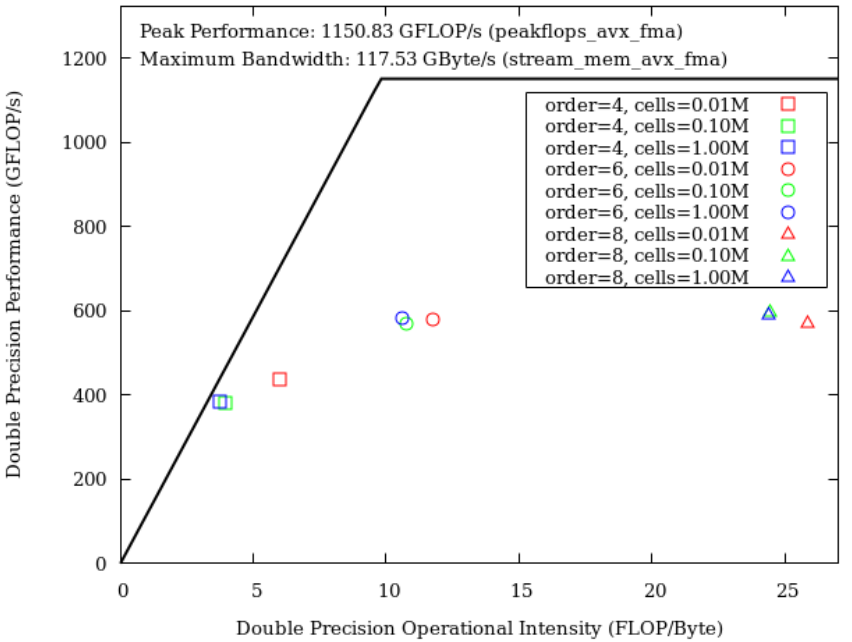
- Theoretical peak FLOPS:
  - Cores
  - Instruction width
  - FMA
  - IPC
  - Maximum clock frequency

- The theoretical maximum memory bandwidth is obtained from Intel's documentation.

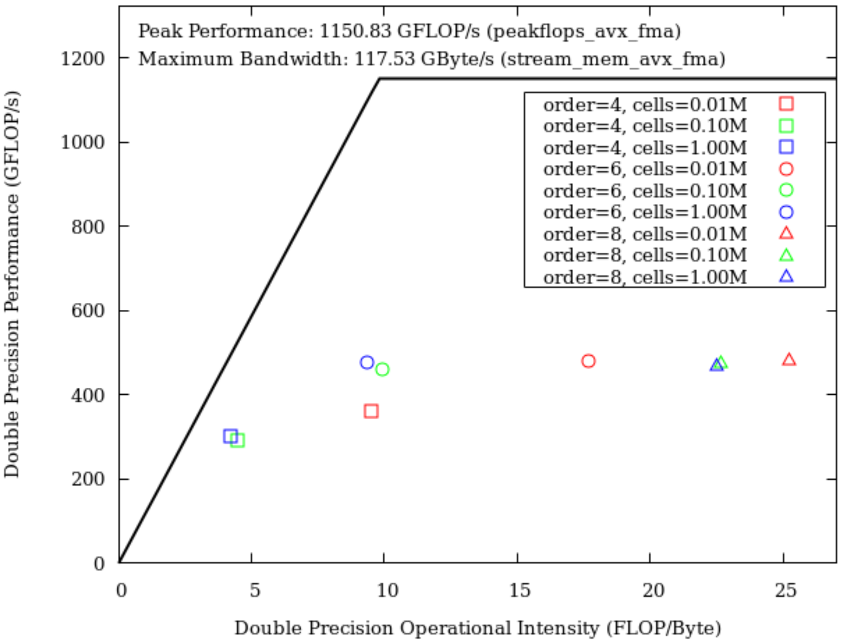


Roofline Models: Elastic vs Acoustic Materials

Elastic ($\mu = 0$):



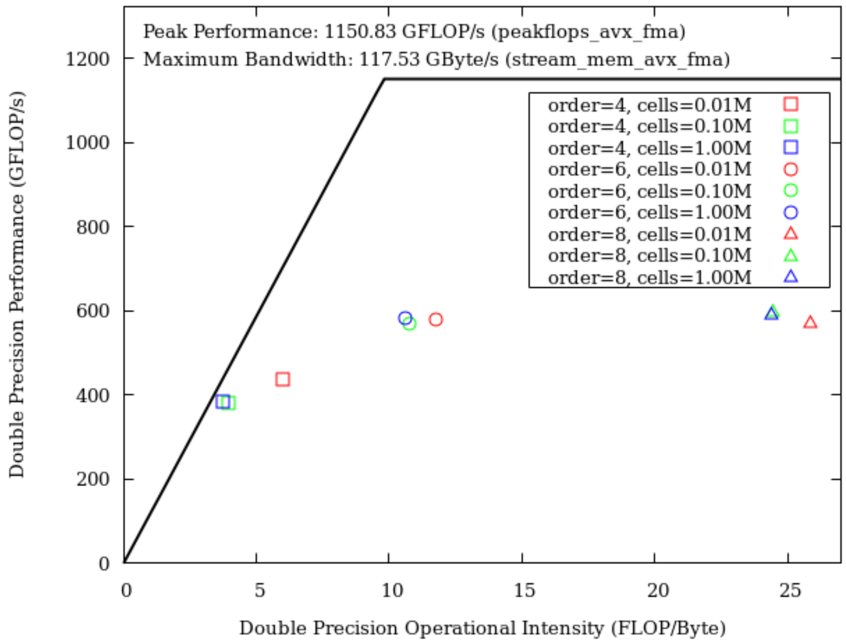
Acoustic:



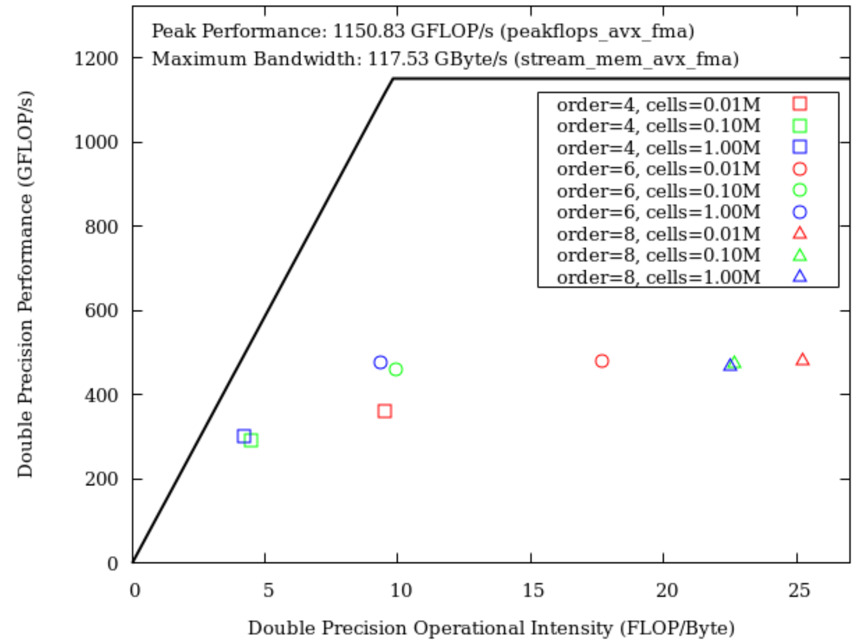
- Is the application compute-bound or memory-bound?
  - Determined by the operational intensity
  - Theoretically, the operational intensity is determined by the code uniquely even without running the program

Roofline Models: Elastic vs Acoustic Materials

Elastic ($\mu = 0$):



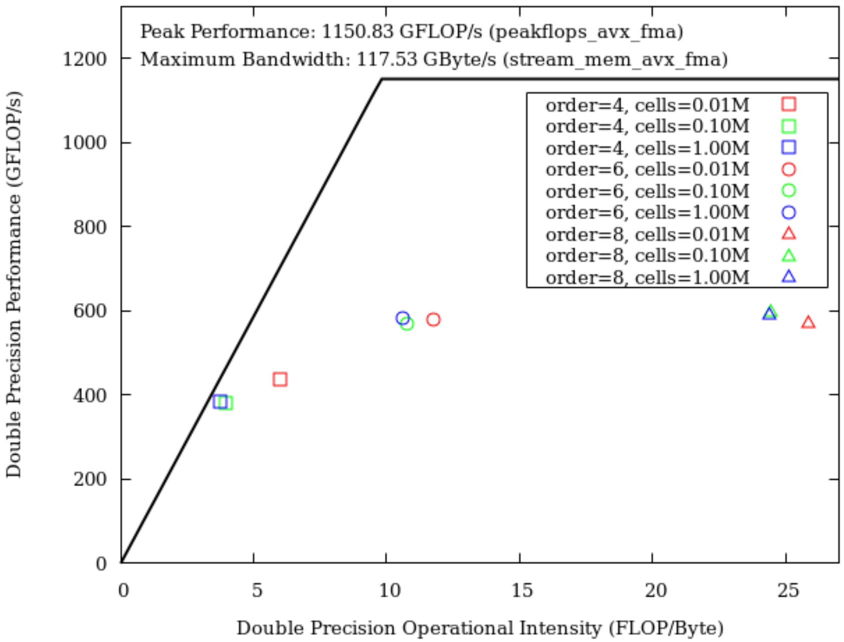
Acoustic:



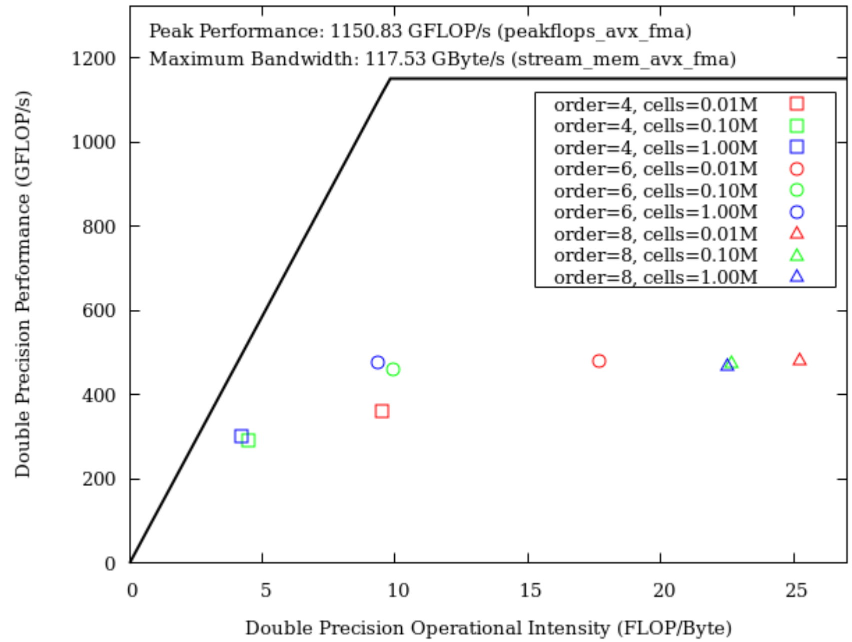
- What is the potential maximum performance for the application, and how to optimize?
  - Moving right: optimizing memory access patterns, reducing unnecessary memory accesses, making better use of caching, efficiently utilizing the cache hierarchy, or compressing data to reduce the amount of data transferred

Roofline Models: Elastic vs Acoustic Materials

Elastic ($\mu = 0$):



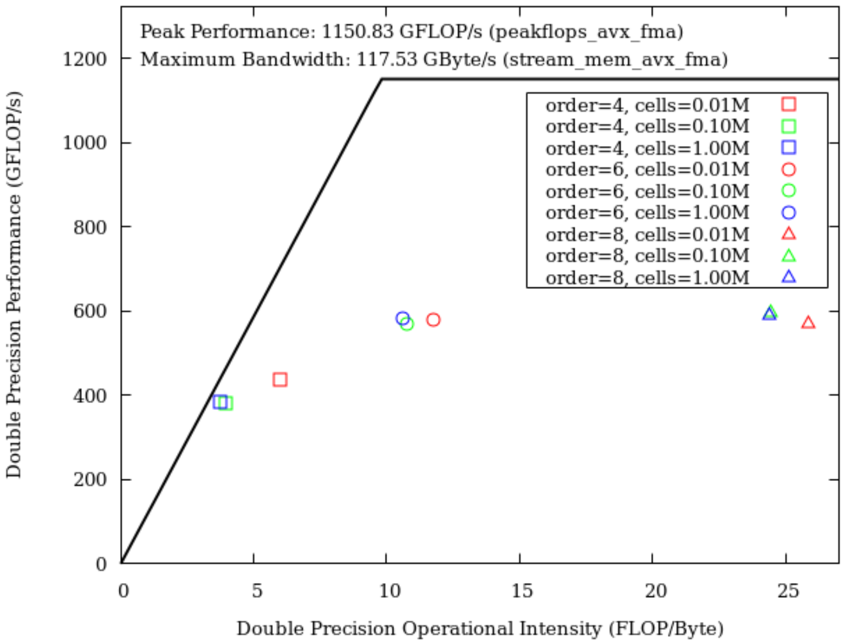
Acoustic:



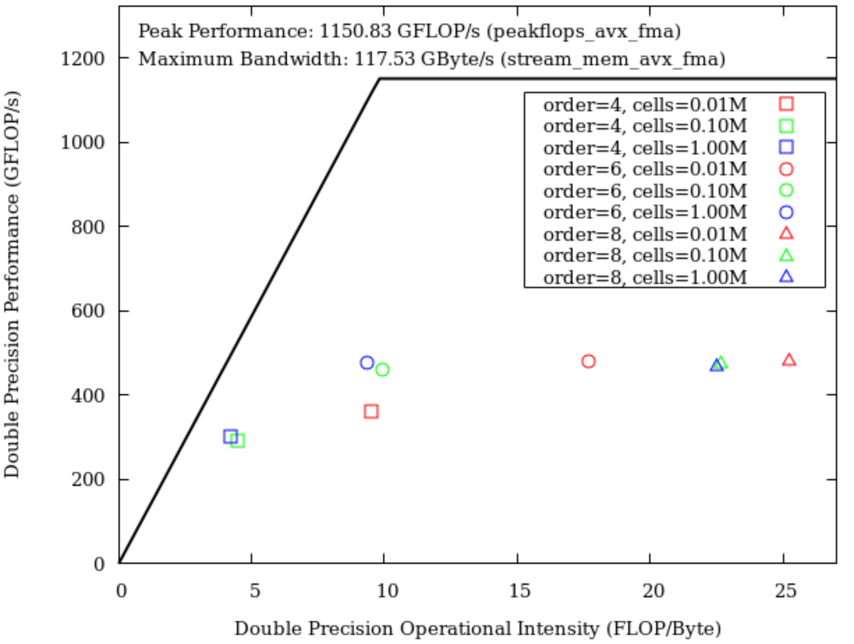
- What is the potential maximum performance for the application, and how to optimize?
  – Moving upward: increasing parallelism, vectorization, using more efficient mathematical algorithms, or leveraging hardware features such as SIMD and FMA instructions to improve computational efficiency

Roofline Models: Elastic vs Acoustic Materials

Elastic ($\mu = 0$):



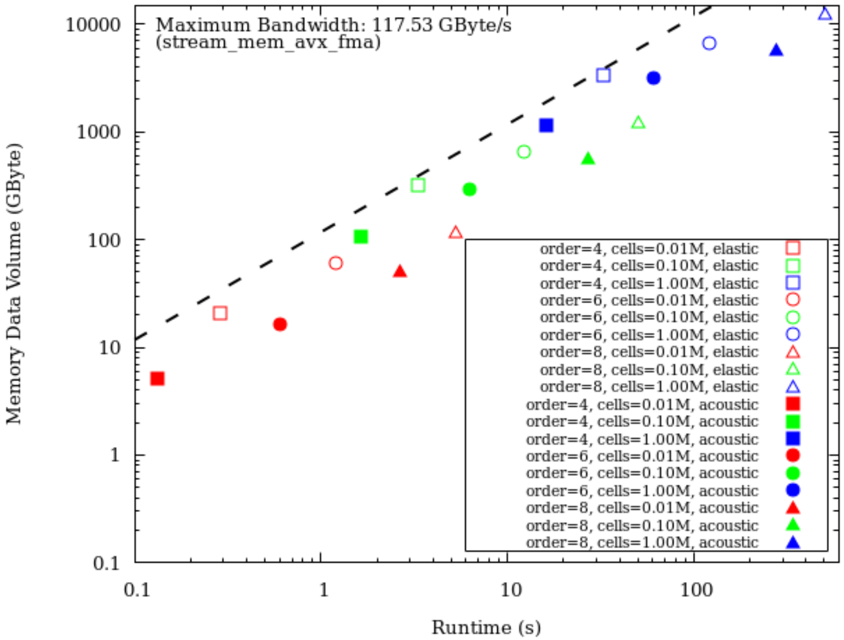
Acoustic:



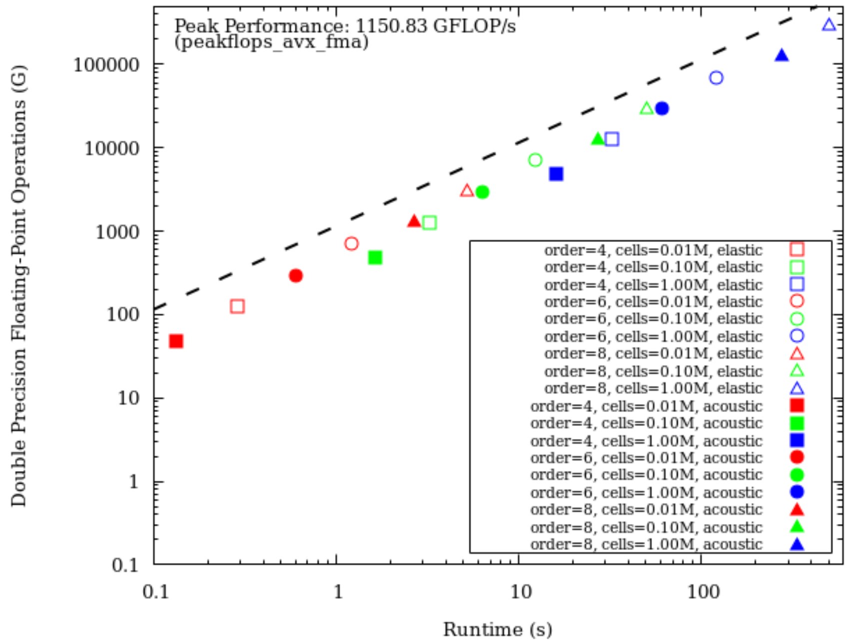
- What is the potential maximum performance for the application, and how to optimize?
  - Upgrading the hardware: memory or processor

Behind Roofline Models

Memory Data Volume vs Runtime:



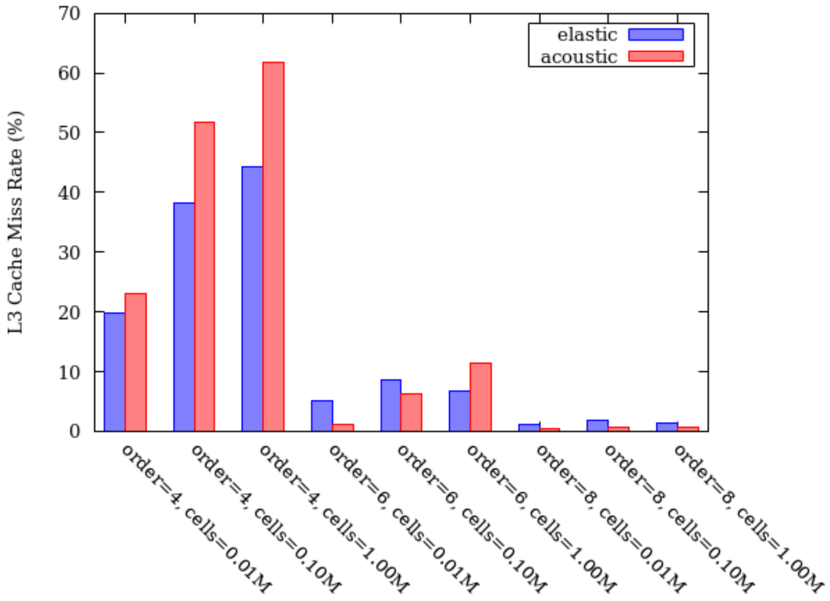
GFLOP vs Runtime:



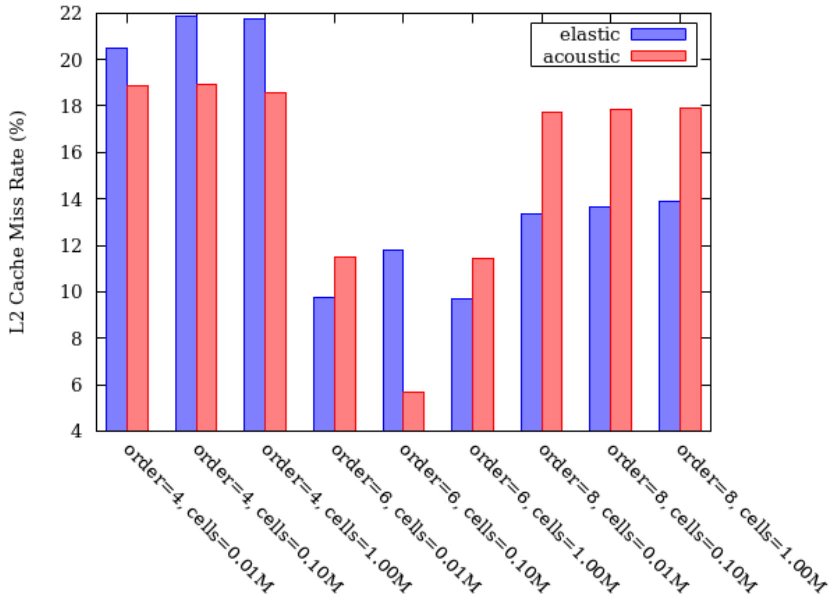
- Memory data volume and runtime are both reduced by approximately half.
- Both FLOPS and memory bandwidth decrease (operational intensity = FLOPS / bandwidth).

L3 and L2 Cache Miss Rates

L3 Cache:



L2 Cache:



Conclusion

- The performance bottlenecks have not significantly changed.
- The memory data volume and runtime have been reduced by approximately half.
- The cache miss rate shows increases and decreases under different test conditions.
- Limitations of roofline model:
  - Simplified assumptions, such as ideal memory access patterns and computational models
  - Missing subtle performance characteristics like memory access latency, cache effects, or thread contention
  - Depending on accurate performance measurements and system parameters
  - Static model
  - Applicability

Future Work

- Implementing the 4-DOF acoustic model for the full version of SeisSol is feasible!
- Performance modeling for distributed memory systems -- 3D “roofline” model?
- Roofline model for heterogeneous computing systems (e.g., CPU+GPU)?

References

Main references for the presentation:

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- https://seissol.readthedocs.io/en/latest/index.html
- https://doku.lrz.de/linux-cluster-10745672.html
- https://github.com/RRZE-HPC/likwid/wiki/Tutorial%3A-Empirical-Roofline-Model

The full list is presented in my report.

THANKS

Questions? Comments?