Performance Portability and Evaluation of Heterogeneous Components of SeisSol Targeted to Upcoming Intel HPC GPUs

Computational Sciesmology with SYCL

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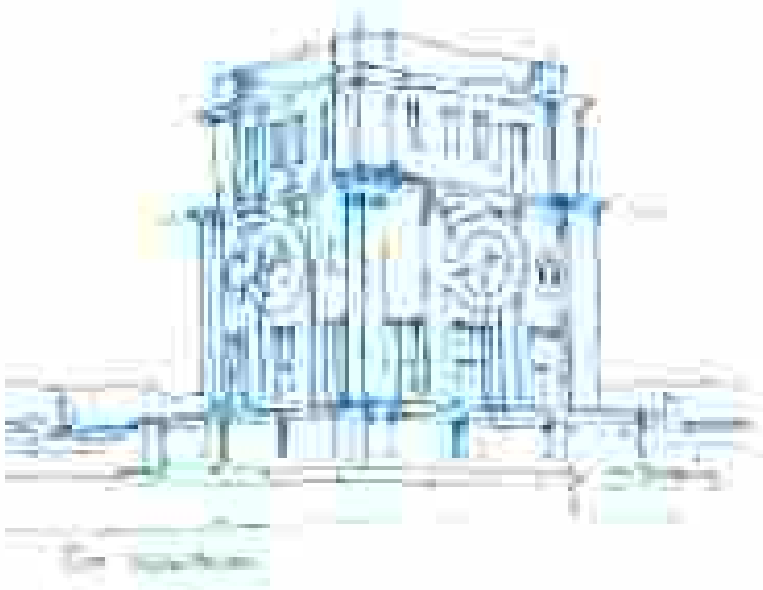


oneAPI Dev Summit, Virtual Conference

Outline of talk

Introduction

GPU computing in SeisSol

SYCL Integration into SeisSol

Performance Evaluation

Simulations with oneAPI

Continuous Integration

Conclusion & Future Work

NOTE:

Illustrations and results without annotations are mostly taking from [2] and [1]

What is SeisSol?

SeisSol - software for simulating seismic waves and earthquake dynamic

based on:

- Discontinious Galerking method
- ADER time-integration scheme
- Tetrahedral meshing

supports:

- Elastic and visco-elastic wave propagation models
- Plasticity model
- Local and Global Time-Stepping schemes
- Point sources and rupture surfaces to model source terms
- Fused-simulations

originally came with:

- MPI+OpenMP parallelization
- Code generator - YATeTo DSL. [3]

ADER-DG in a Nutshell

Update Scheme

$$Q_k^{n+1} = Q_k^n + M^{-1}(K^\xi D_\xi A_k^* + K^\eta D_\eta B_k^* + K^\zeta D_\zeta C_k^*) \tag{1}$$

$$- \frac{1}{|J|} M^{-1} \left(\sum_{i=1}^{4} |S_i| F^{-,*} D_\chi \bar{A}_k^i \right)$$

$$- \frac{1}{|J|} M^{-1} \left(\sum_{i=1}^{4} |S_i| F^{-,*} A_{k(i)} D_{k(i)} \bar{A}_{k(i)} \right)$$

Cauchy-Kowalewski

$$\bar{D}_k = \sum_{i=0}^{O-1} \frac{(t^{n+1} - t^n)^{i+1}}{(i+1)!} \frac{\partial^i}{\partial t^i} Q_k^n \tag{2}$$

$$\frac{\partial^{i+1}}{\partial t^{i+1}} Q_k^n = M^{-1} \left[(K^\xi)^T \left(\frac{\partial^i}{\partial t^i} Q_k^n \right) A_k^* + (K^\eta)^T \left(\frac{\partial^i}{\partial t^i} Q_k^n \right) B_k^* + (K^\zeta)^T \left(\frac{\partial^i}{\partial t^i} Q_k^n \right) C_k^* \right] \tag{3}$$

Source Code Structure and Code Generation with YATeTo

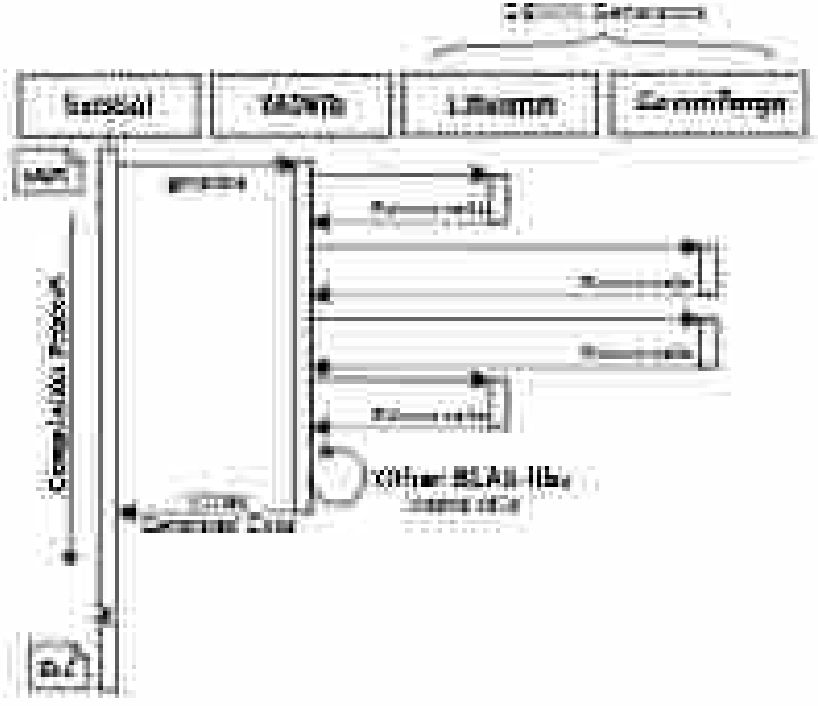


Figure: Compilation process

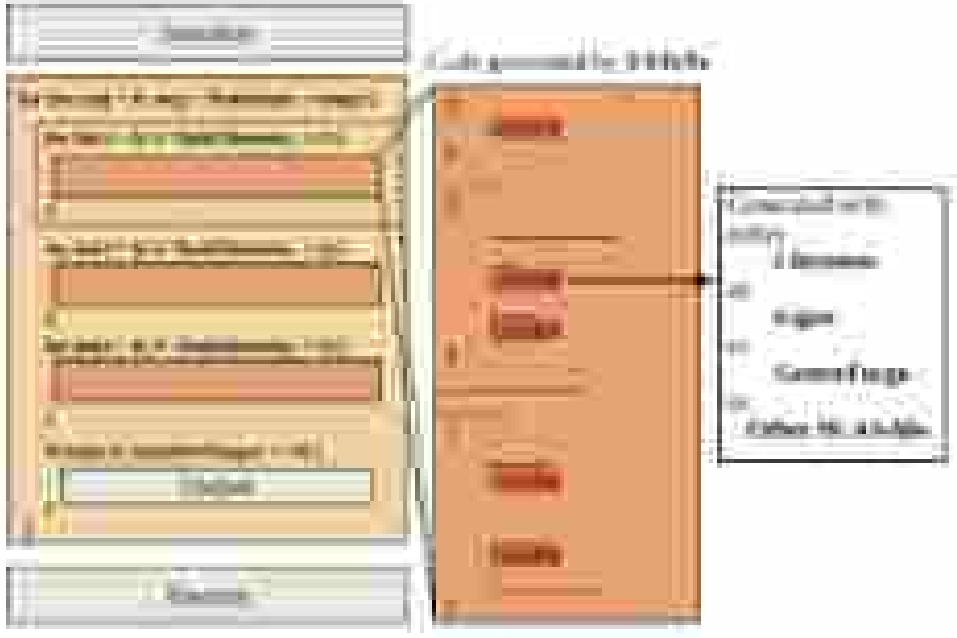


Figure: Simplified source code structure

```
volumeSum = self.Q['kp']
for i in range(3):
  volumeSum += self.db.kXiiM[i][self.t('kl')] * self.I['iq'] * self.starMatrix[i]['qp']

volume = (self.Q['kp'] <= volumeSum)
generator.add('volume', volume)
```

Listing: Example of YATeTo DSL

GPU computing in SeisSol

Figure: CPU/GPU task parallelism

Binary Batched Operations:

- Trivial grid/block distribution
- Easy to estimate run-time resources i.e., shared memory, registers

But:

- Finer granularity w.r.t CPU-like parallelism
- Lower arithmetic intensity

GemmForge on Nvidia V100

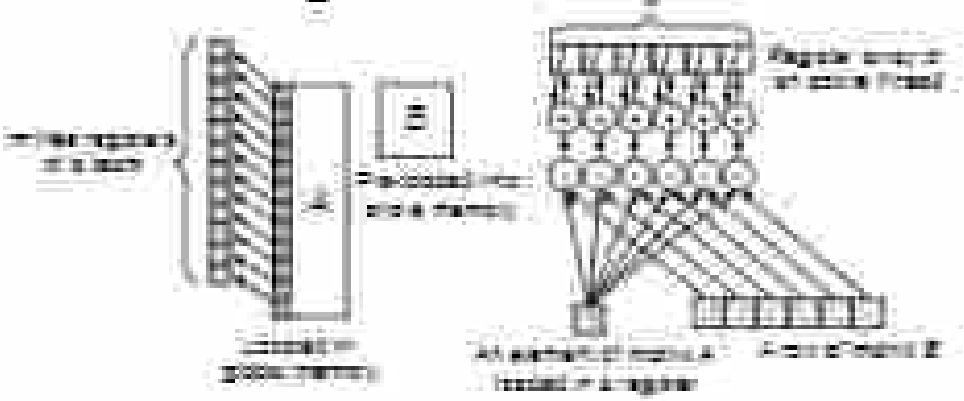
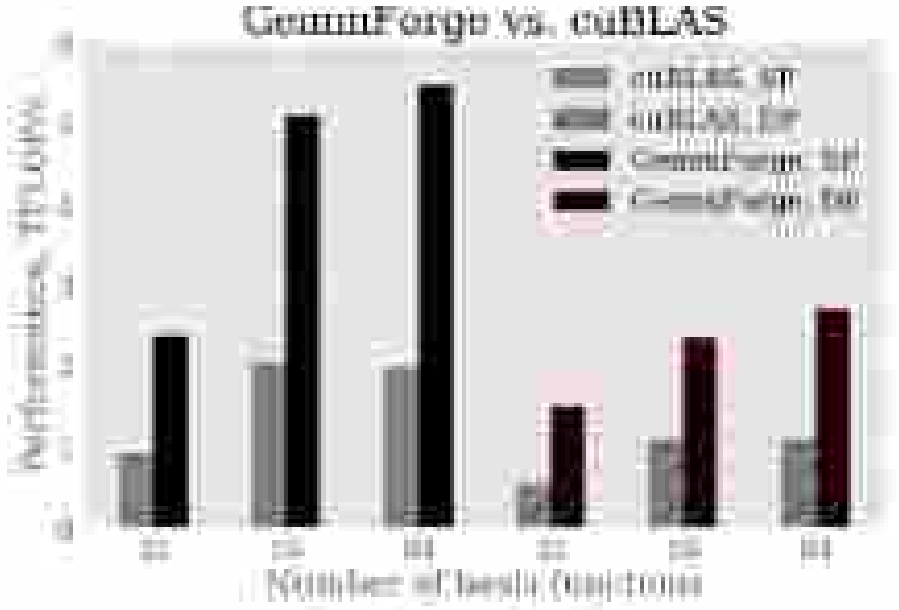


Figure: Sum of parallel outer products



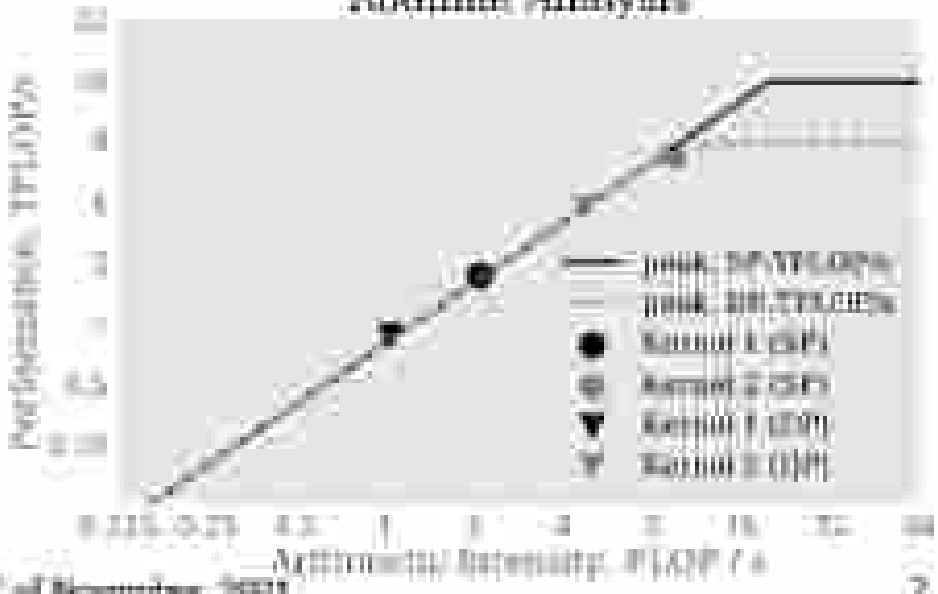
Benchmark:

$$L_e = D \cdot A_e \cdot B_e + L_e \tag{4}$$

where $L_e A \in \mathbb{R}^{n \times 9}$ and $B \in \mathbb{R}^{9 \times 9}$, $D \in \mathbb{R}^{n \times n}$ represents either a mass or stiffness matrix.

Implementation:

$$T_e = A_e \cdot B_e$$
$$L_e = D \cdot T_e + L_e \tag{5}$$



Weak Scaling on Marconi 100

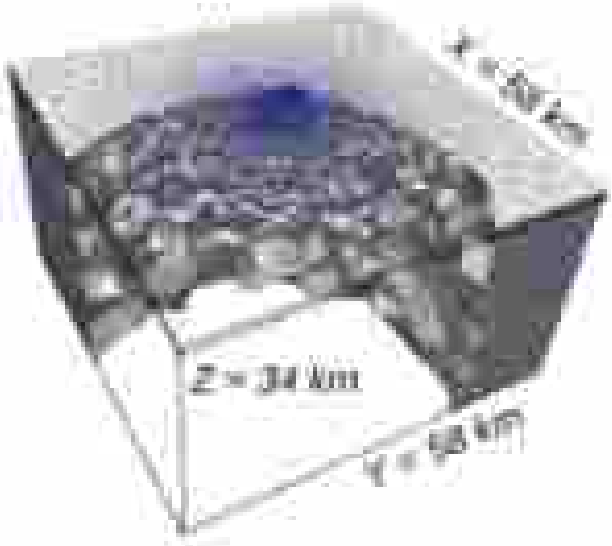
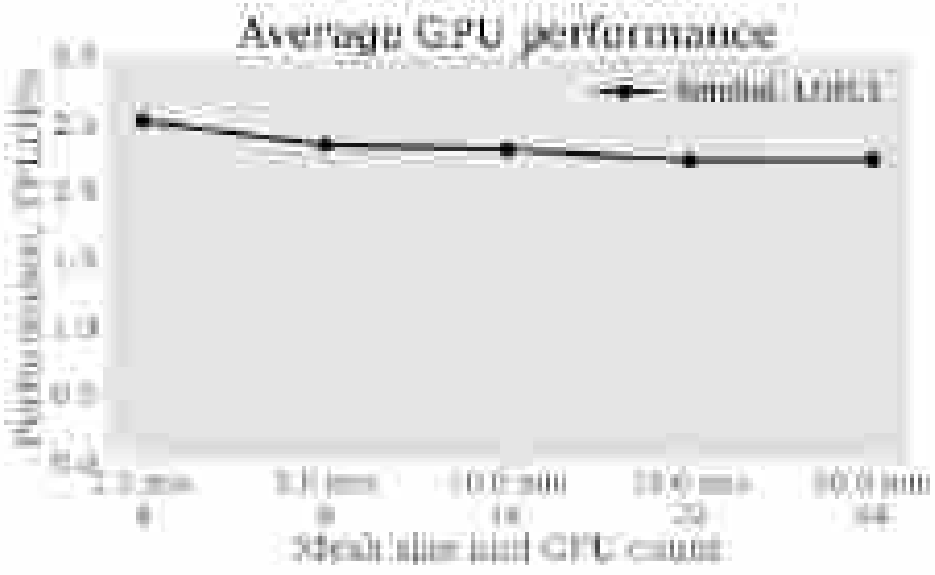


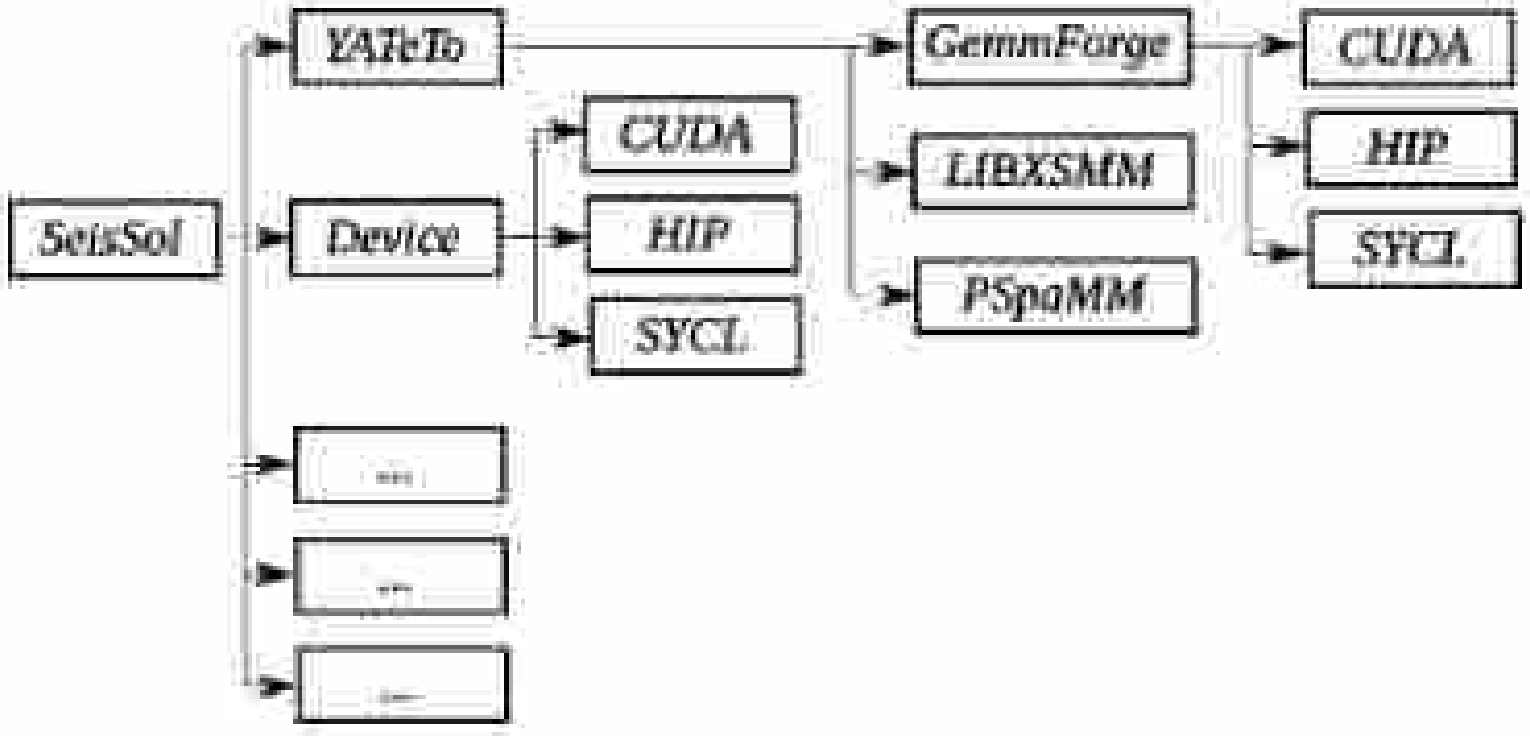
Figure: Layer Over Half space (LOH)

- Parameterized CAD model
- Single point source
- 2 layers with different materials



But SeisSol has some problems with Strong Scaling on GPUs

SeisSol Structure

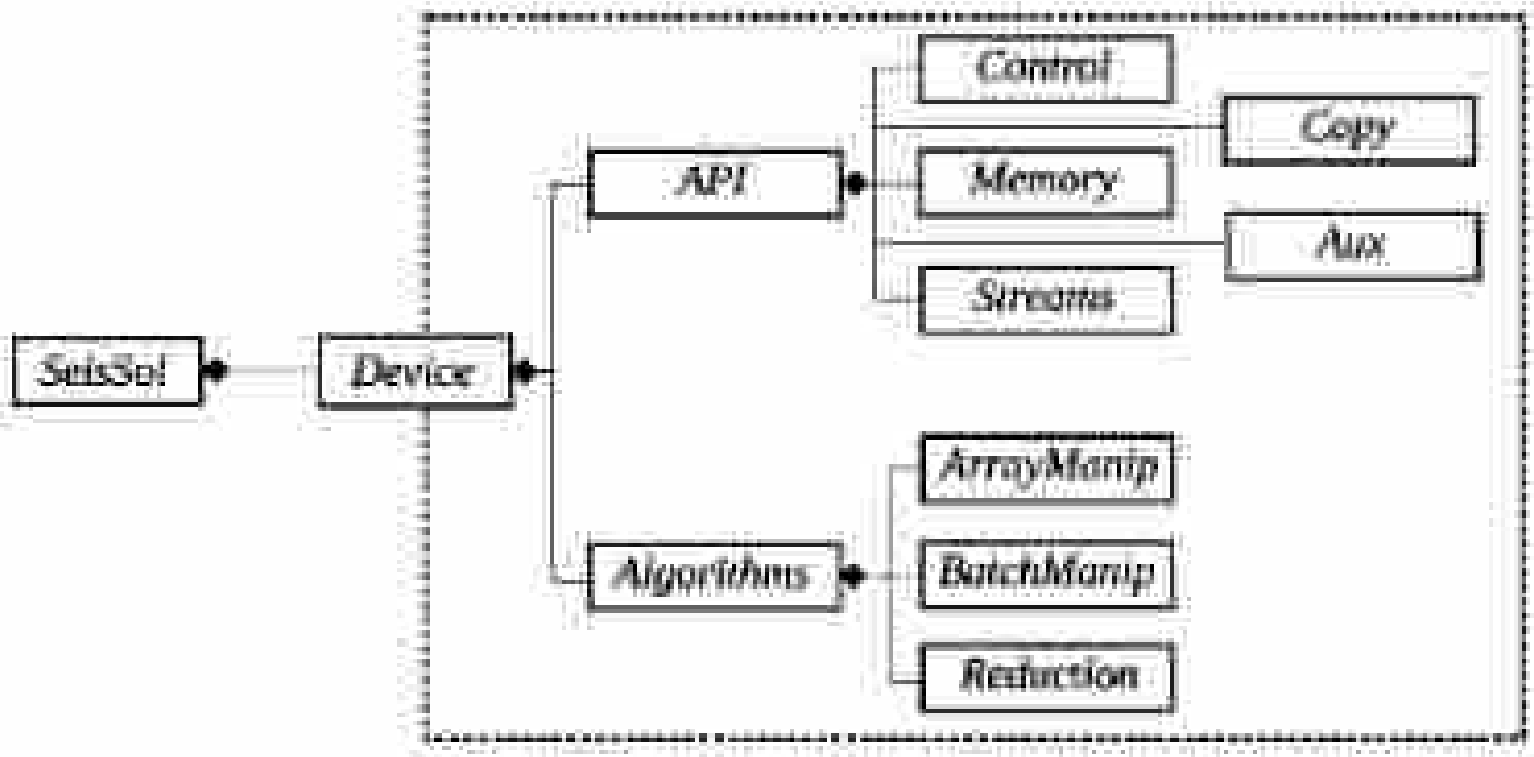


SYCL is a subset of DPC++

- Open language from the Khronos group

Device

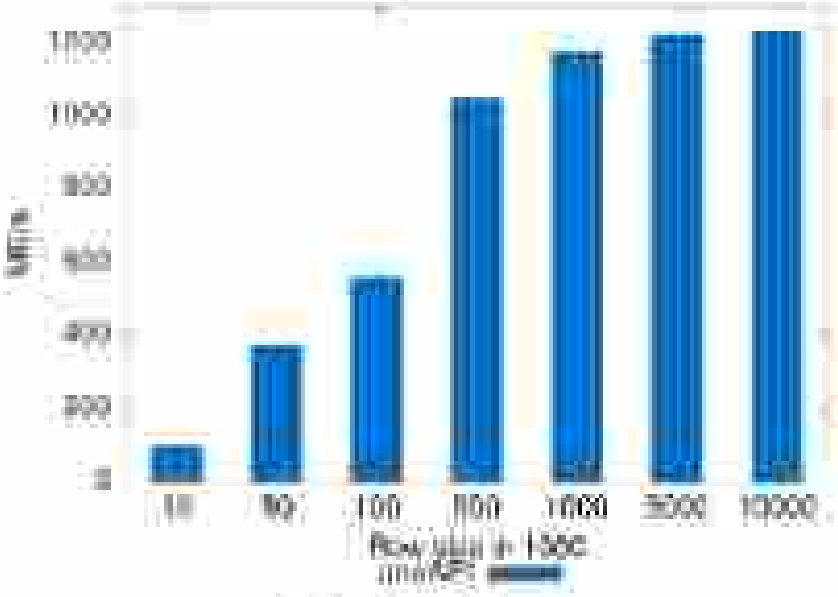
- Provides a simplified interface to GPUs
- Adapts specific GPU APIs and algorithms
- Separate compilation of CPU and GPU source codes
  - ! No GPU specific data types in SeisSol



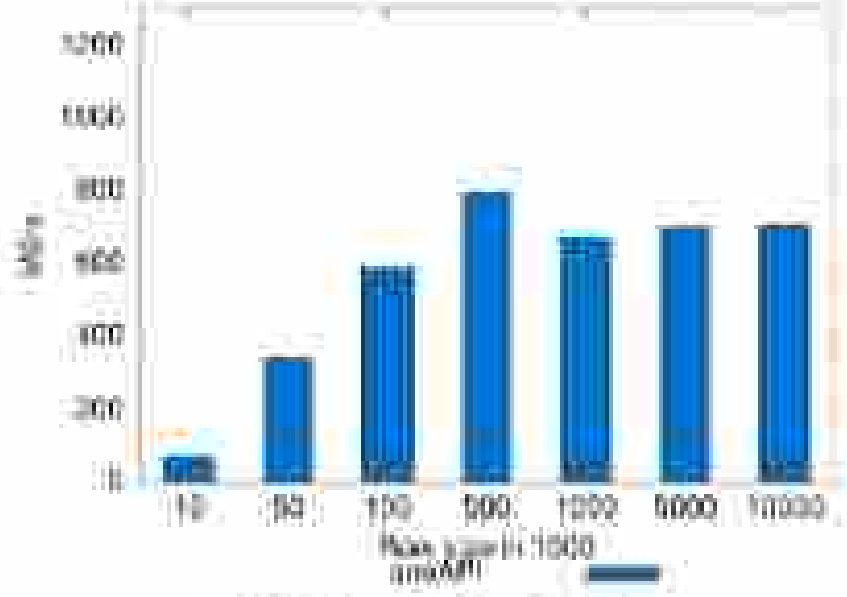
Parallel Jacobi Benchmark (PJB)

- Approximation of a system of linear equations $Ax = b$
- Fix point iteration algorithm
- Parallel implementations GEMV and AXPY on GPUs
- Uses collectives of GPU-Aware MPI
- Uses Device API i.e., *Control*, *Memory* and *Copy* components
- Measures throughput in MB/s for Computations and Communication

Computational Throughput



Iris Xe Max

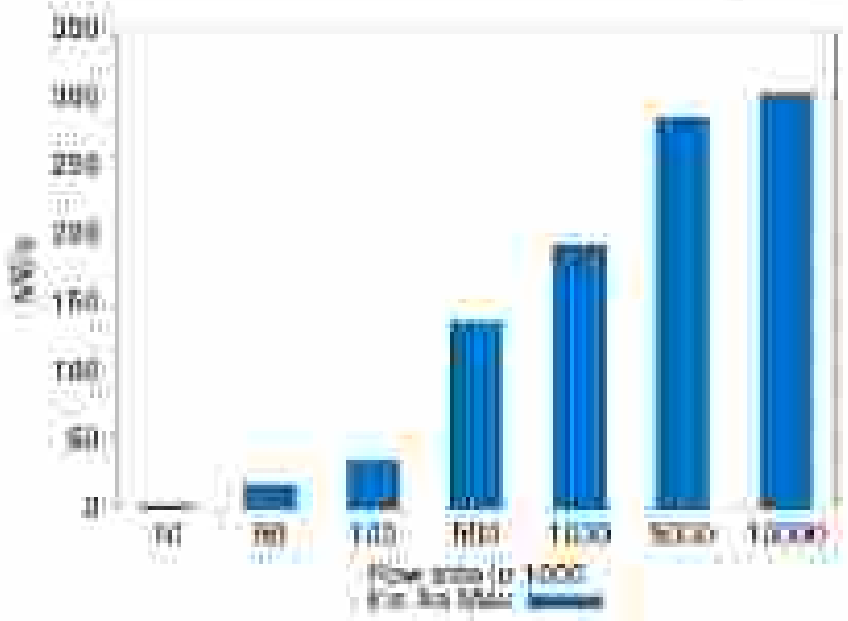


UHD Graphics P630

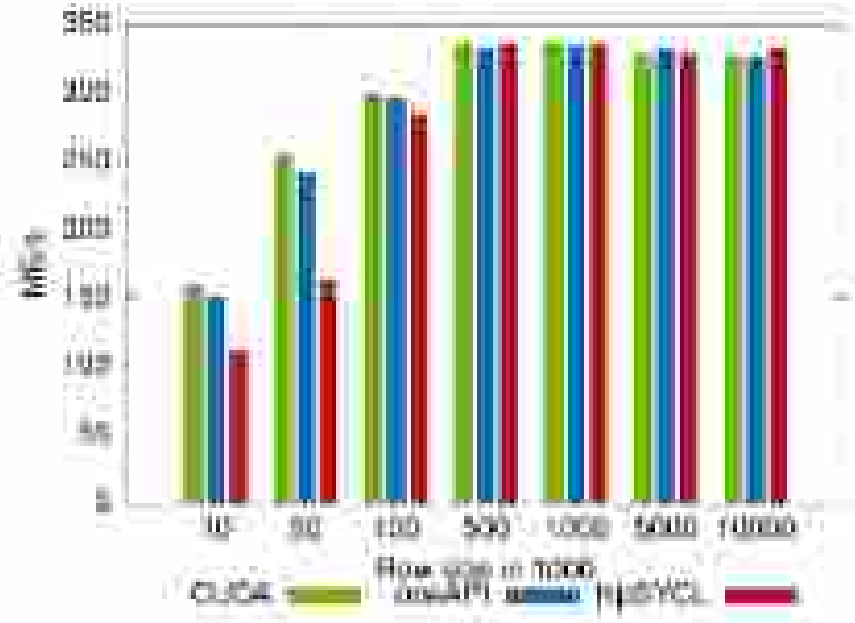
PJB — Communicational Throughput

Intel MPI vs. OpenMPI with 2 GPUs

- Performance of Intel GPU-Aware MPI is not going affect SeisSol
- SeisSol relies on non-blocking P2P communication



Iris Xe Max - Intel MPI



RTX3090 - OpenMPI

GemmForge

$$T_e = A_e \cdot B_e \tag{6}$$

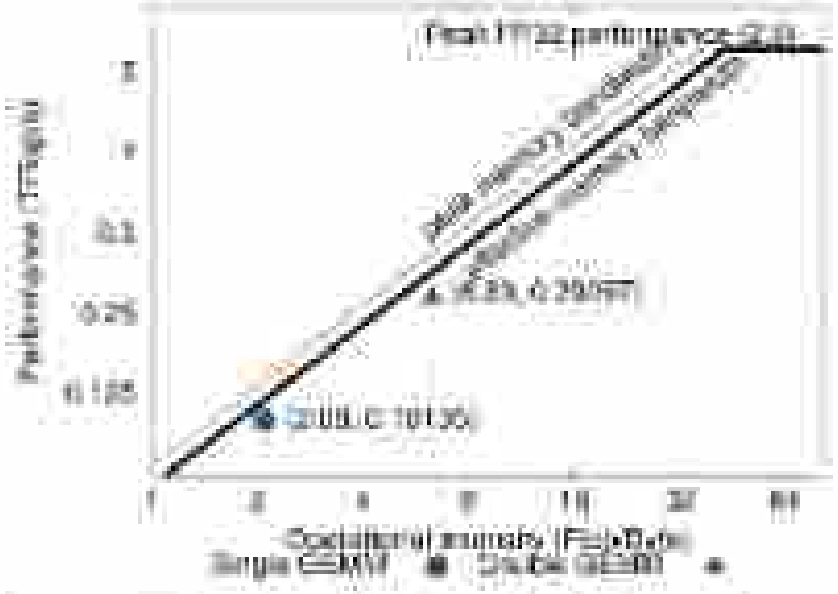
$$L_e = D \cdot T_e + L_e \tag{7}$$

where $L_e, A_e \in \mathbb{R}^{56 \times 8}$, $B_e \in \mathbb{R}^{8 \times 9}$, $D \in \mathbb{R}^{56 \times 56}$

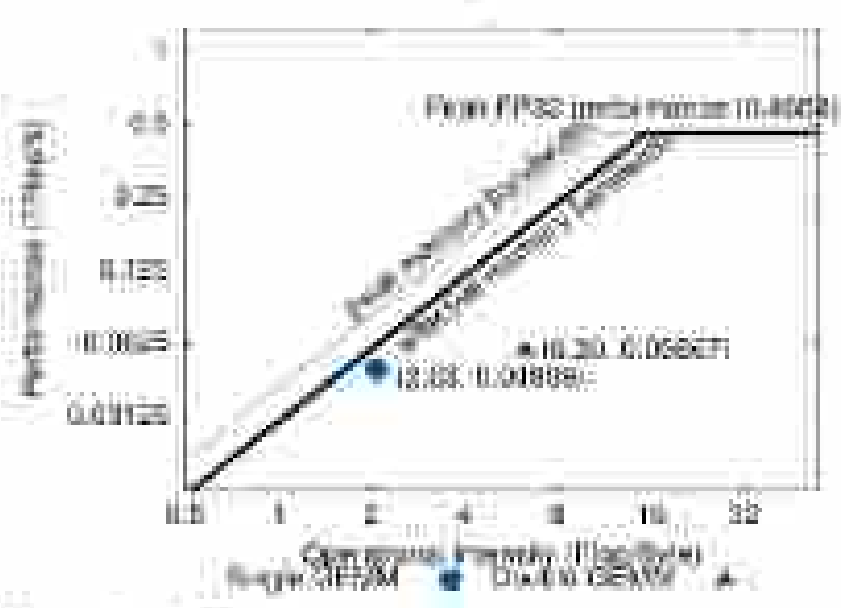
GemmForge Benchmark specification:

- Single GEMM: Equation 6
- Double GEMM: Equations 6 and 7

Intel Iris Xe

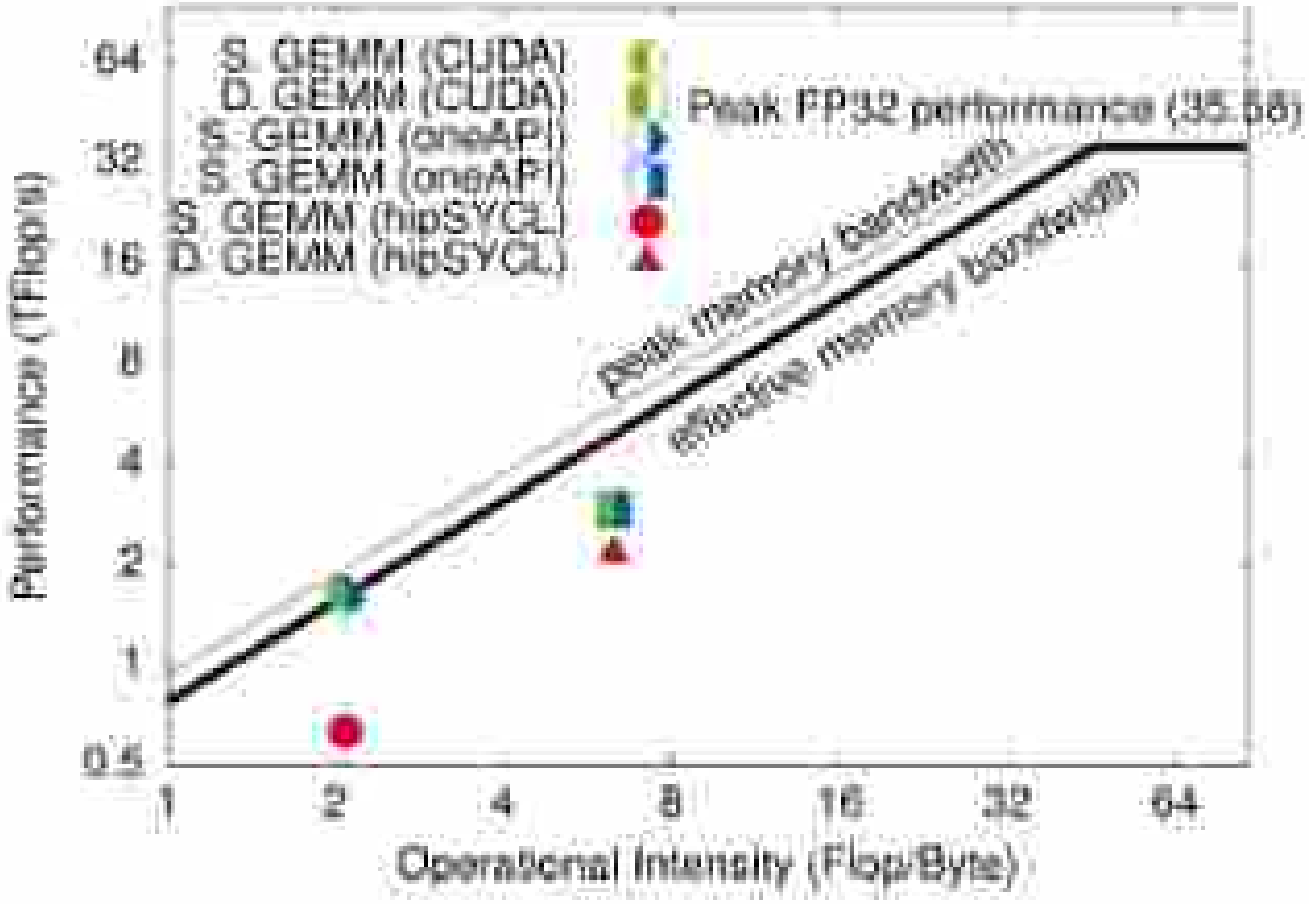


Intel UHD Graphics P630



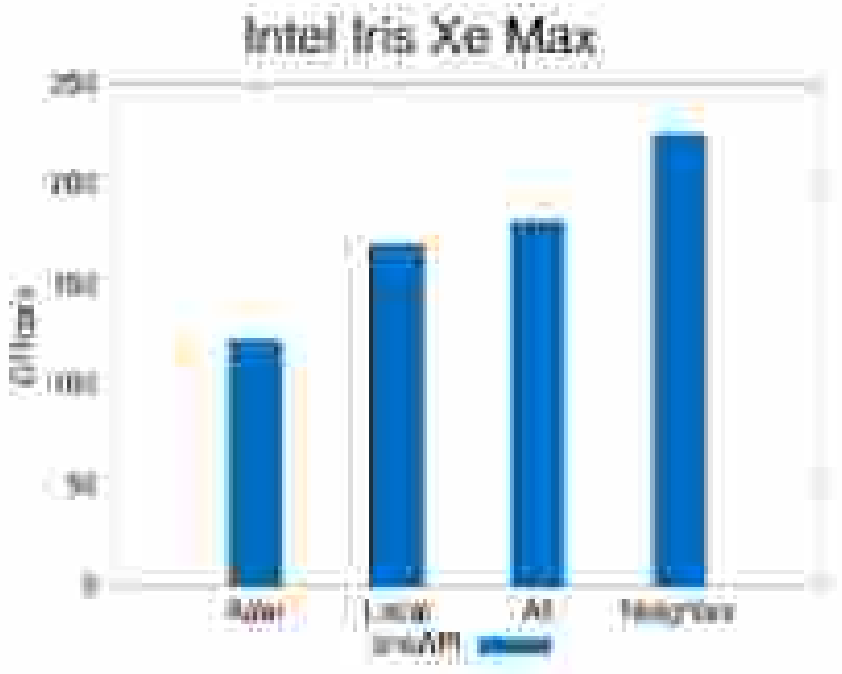
GemmForge

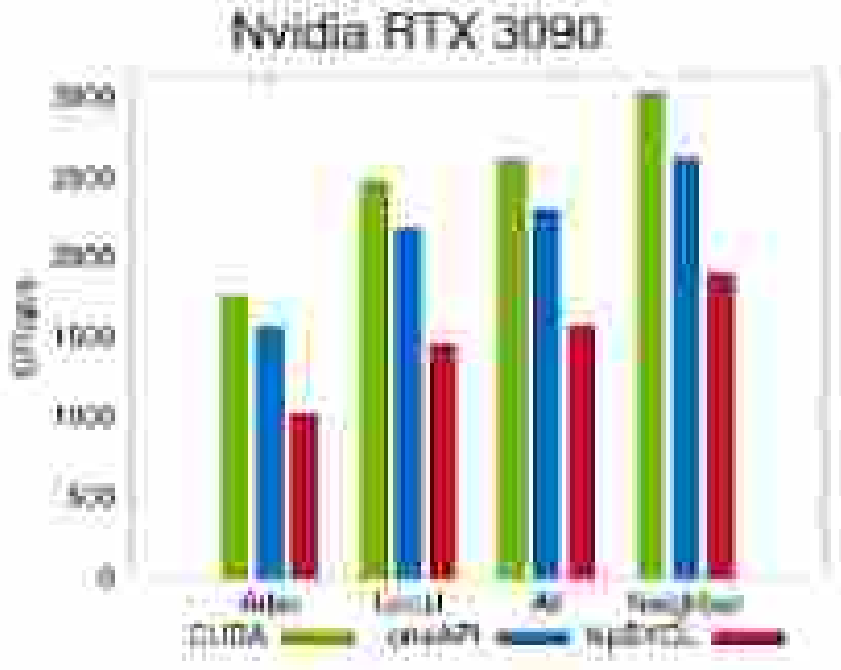
Nvidia RTX 3090 Turbo



SeisSol Proxy

- Contains main computational macro-kernels
- Based on a single time cluster
- Allows to test:
  - Individual macro-kernels
  - Combinations of them





Simulations: LOH.1

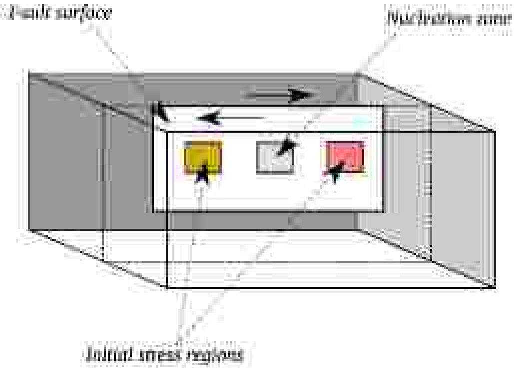
- 2 RTX3090 Turbo GPUs using in a single node
- Using CUDA-Aware OpenMPI via UCX
- Single MPI process per GPU
- Using a dedicated communication thread per MPI process
- Compiled with DPCPP
- Mesh with 1 million elements

Achieved:

- Correct numerical results
- Expected performance based on benchmark results

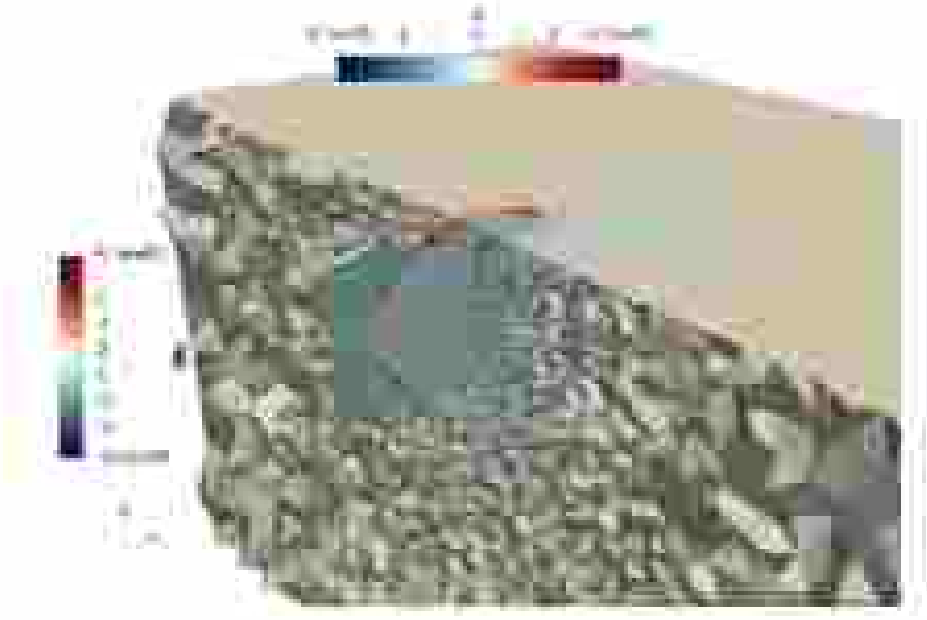
Simulations: TPV5

- Vertical strike-slip fault in homogeneous half-space
- Rupture is artificially nucleated in a square zone at the center
- Two square patches with initial stress conditions
  - higher on the left
  - lower on the right



Simulations: TPV5

- Using the same hardware setup as for LOH.1
- Computing Dynamic Rupture on CPU using all available cores
- Mesh with 2 million elements



Achieved:

- Correct numerical results
- Expected performance

SeisSol CI

- Added SYCL to *SeisSol Device*, *GemmForge* CI pipelines
- Testing SYCL with hipSYCL
- Docker containerization for reproducibility
- CI runner equipped with a single Nvidia TITAN Xp

Conclusion & Future Work

Conclusion:

- Managed into integrate SYCL model into SeisSol
- Correct numerical results
- Expected performance on RTX 3090
- Worked with only 2 isolated components i.e, *Device*, *GemmForge*
- SYCL may replace *Device* in a long-term future

Future work:

- Merging to SeisSol's master branch
- Improving SeisSol building system
- Integrating SYCL into *ChainForge* fused-GEMM generator
- Implementing static SeisSol GPU code with OpenMP offloadings
  - Plasticity model
  - Dynamic rupture

References I

[1] Ravil Dorozhinskii and Michael Bader. "SeisSol on Distributed Multi-GPU Systems: CUDA Code Generation for the Modal Discontinuous Galerkin Method". In: *The International Conference on High Performance Computing in Asia-Pacific Region*. 2021, pp. 69–82.

[2] Kratul Ludwig. "Performance Portability and Evaluation of Heterogeneous Components of SeisSol Targeted to Upcoming Intel HPC GPUs". Bachelorarbeit. Technical University of Munich, 2021.

[3] Carsten Uphoff and Michael Bader. "Yet Another Tensor Toolbox for discontinuous Galerkin methods and other applications". en. In: *ACM Transactions on Mathematical Software* 46.4 (2020). DOI: 10.1145/3406835.