High-Performance Earthquake Simulation on Xeon Phi Platforms

Perspectives of GPU Computing in Science

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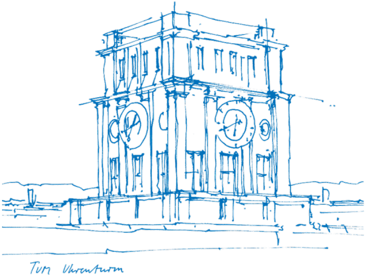
Rome, 27 Sep 2016



Overview and Agenda

Dynamic Rupture and Earthquake Simulation with SeisSol:

- unstructured tetrahedral meshes
- high-order ADER-DG discretisation
- compute-bound performance via optimized matrix kernels

Optimising SeisSol for Xeon Phi Platforms

- offload scheme: 1992 Landers Earthquake as landmark simulation, scalability on SuperMUC, Tianhe-2, Stampede
- optimisation for Knights Corner and Landing
- towards simulations in symmetric mode (1st results on Salomon)

Part I

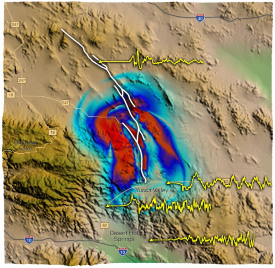
Dynamic Rupture and Earthquake Simulation with SeisSol

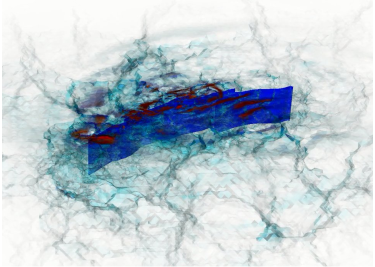
`http://www.seissol.org/`

Dumbser, Käser et al. [9]
An arbitrary high-order discontinuous Galerkin method . . .

Pelties, Gabriel et al. [11]
Verification of an ADER-DG method for complex dynamic rupture problems

Dynamic Rupture and Earthquake Simulation



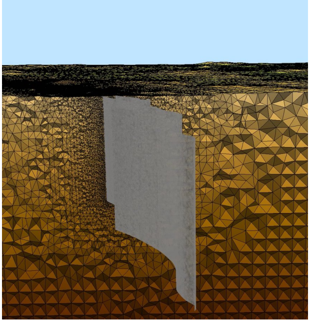


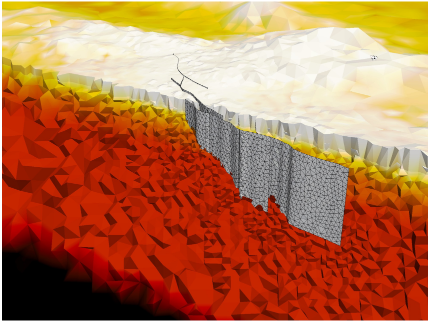
Landers fault system: simulated ground motion and seismic waves [3]

SeisSol – ADER-DG for seismic simulations:

- adaptive tetrahedral meshes
  → complex geometries, heterogeneous media, multiphysics
- complicated fault systems with multiple branches
  → non-linear multiphysics dynamic rupture simulation
- ADER-DG: high-order discretisation in space and time

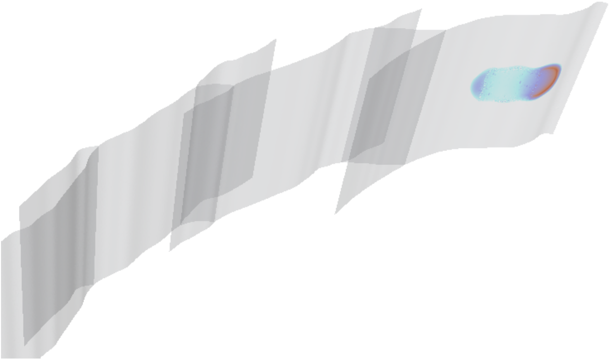
Example: 1992 Landers M7.2 Earthquake





- multiphysics simulation of dynamic rupture and resulting ground motion of a M7.2 earthquake
- fault inferred from measured data, regional topography from satellite data, physically consistent stress and friction parameters
- static mesh refinement at fault and near surface

Multiphysics Dynamic Rupture Simulation



- spontaneous rupture, non-linear interaction with wave-field
- featuring rupture jumps, fault branching, etc.
- tackles fundamental questions on earthquake dynamics
- realistic rupture source for seismic hazard assessment

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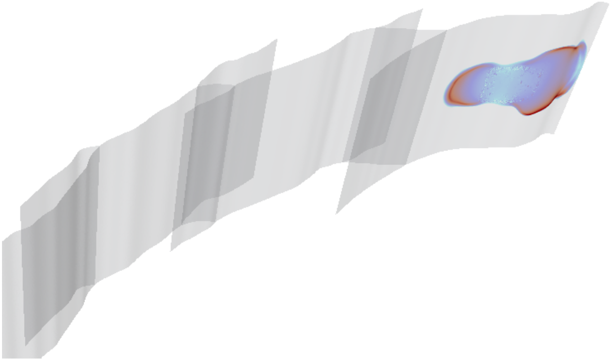

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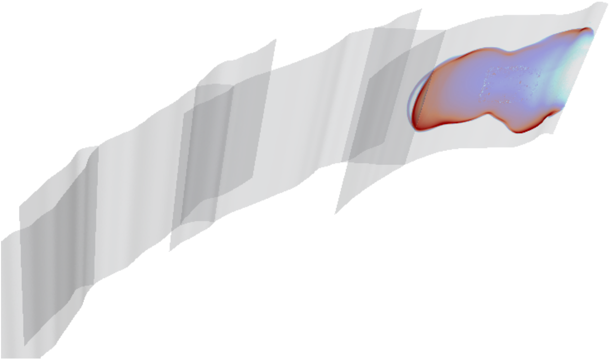

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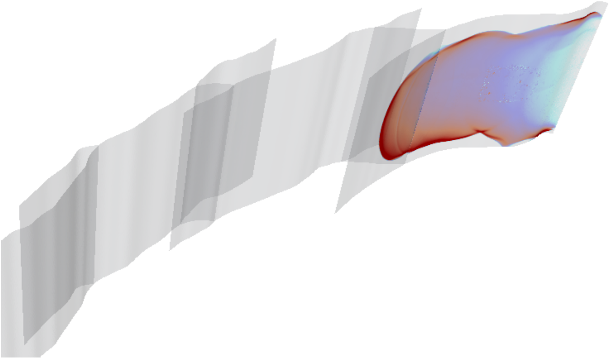

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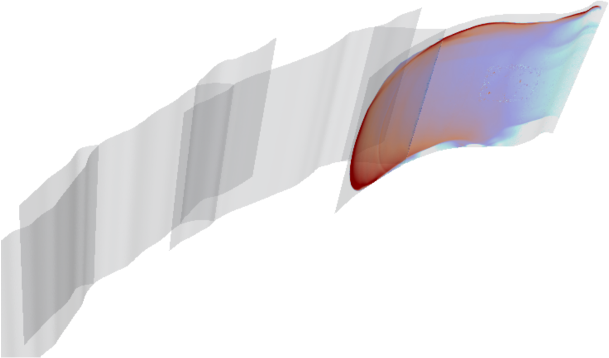

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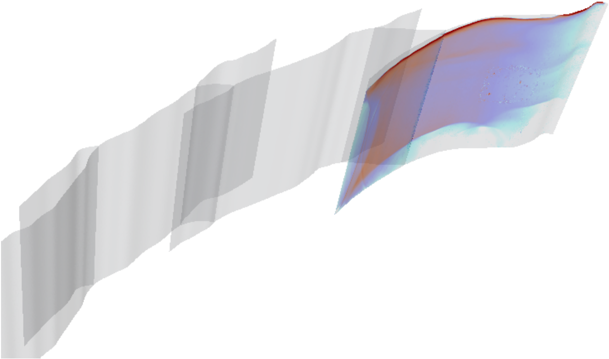

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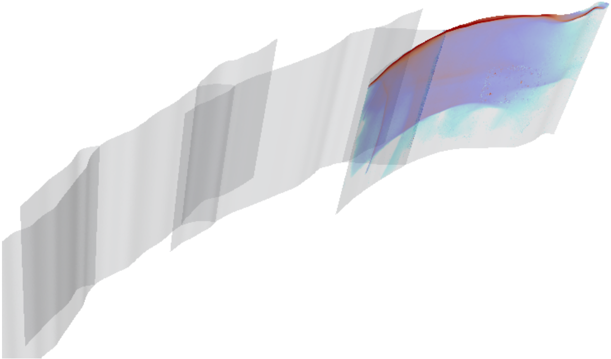

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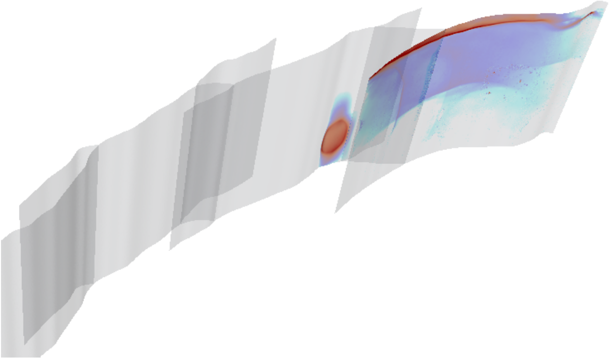

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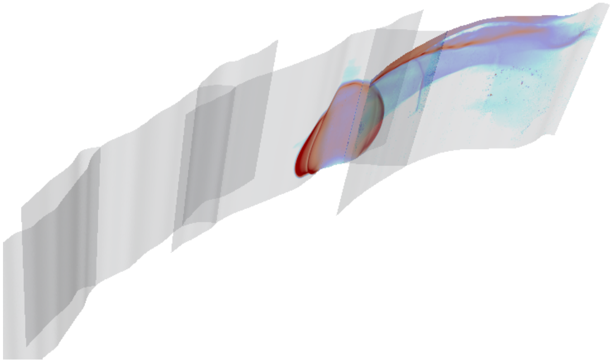

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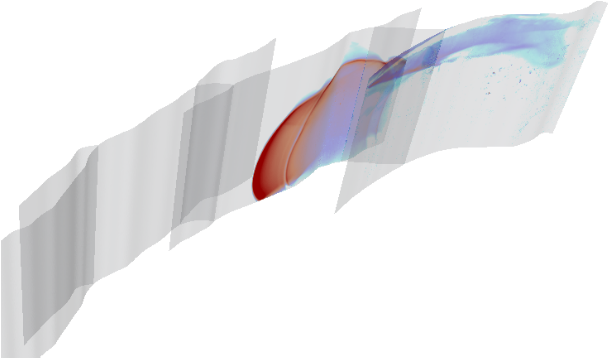

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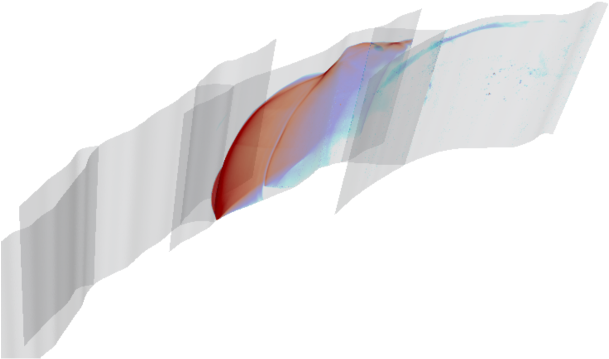

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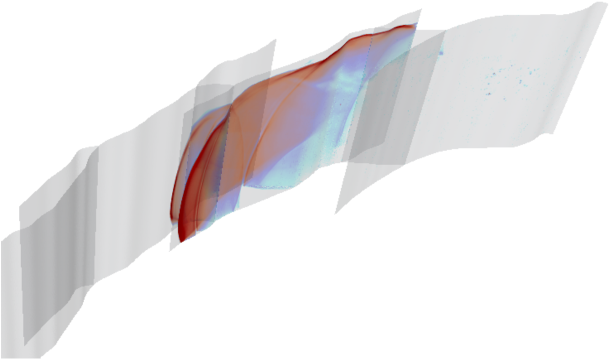

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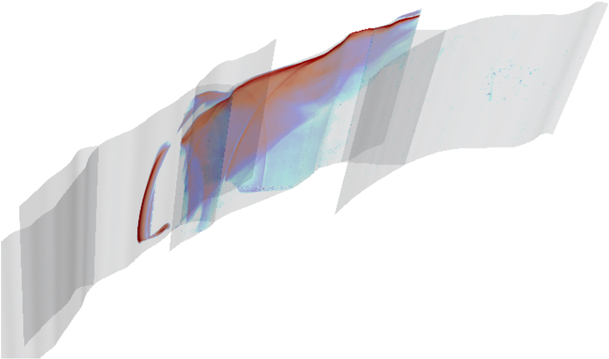

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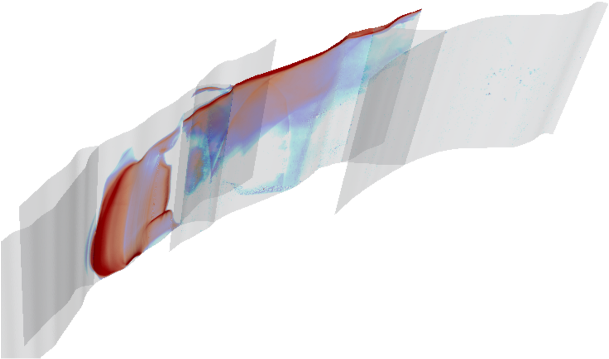

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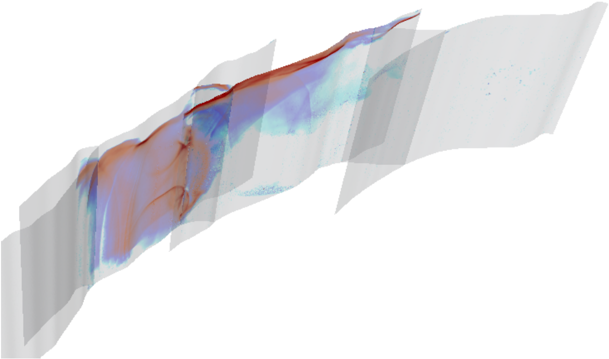

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Part II

SeisSol as a Compute-Bound Code: Code Generation for Matrix Kernels

Breuer, Heinecke, Rannabauer, Bader [1]: High-Order ADER-DG Minimizes Energy- and Time-to-Solution of SeisSol (ISC'15)
Uphoff, Bader: Generating high performance matrix kernels for earthquake simulations with viscoelastic attenuation (HPCS 2016, accepted)

Seismic Wave Propagation with SeisSol

Elastic Wave Equations: (velocity-stress formulation)

$$q_t + Aq_x + Bq_y + Cq_z = 0$$

$$\text{with} \quad q = (\sigma_{11}, \sigma_{22}, \sigma_{33}, \sigma_{12}, \sigma_{23}, \sigma_{13}, u, v, w)^T$$

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & -\lambda - 2\mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\mu \\ -\rho^{-1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\rho^{-1} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -\rho^{-1} & 0 & 0 & 0 \end{pmatrix} \quad B = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda - 2\mu & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\lambda & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -\mu & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -\mu \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\rho^{-1} & 0 & 0 & 0 & 0 & 0 \\ 0 & -\rho^{-1} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\rho^{-1} & 0 & 0 & 0 & 0 \end{pmatrix}$$

- high order discontinuous Galerkin discretisation
- **ADER-DG**: high approximation order in space and time:
- additional features: local time stepping, high accuracy of earthquake faulting (full frictional sliding)

$\rightarrow$ Dumbser, Käser et al., e.g. [9]

SeisSol in a Nutshell – ADER-DG

Update scheme

$$
\begin{aligned}
Q_k^{n+1} = Q_k - \frac{|S_k|}{|J_k|} M^{-1} \Bigg(& \sum_{i=1}^{4} F^{-,i} I(t^n, t^{n+1}, Q_k^n) N_{k,i} A_k^+ N_{k,i}^{-1} \\
& + \sum_{i=1}^{4} F^{+,i,j,h} I(t^n, t^{n+1}, Q_{k(i)}^n) N_{k,i} A_{k(i)}^- N_{k,i}^{-1} \Bigg) \\
& + M^{-1} K^{\xi} I(t^n, t^{n+1}, Q_k^n) A_k^* \\
& + M^{-1} K^{\eta} I(t^n, t^{n+1}, Q_k^n) B_k^* \\
& + M^{-1} K^{\zeta} I(t^n, t^{n+1}, Q_k^n) C_k^*
\end{aligned}
$$

Cauchy Kovalewski

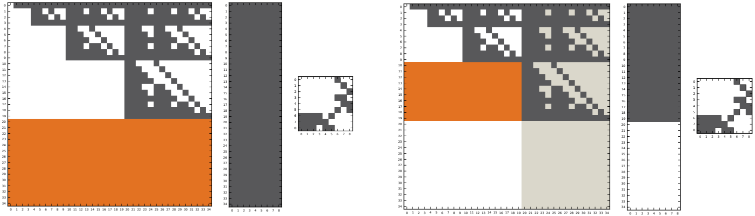
$$
I(t^n, t^{n+1}, Q_k^n) = \sum_{j=0}^{J} \frac{(t^{n+1} - t^n)^{j+1}}{(j+1)!} \frac{\partial^j}{\partial t^j} Q_k(t^n)
$$

$$
(Q_k)_t = -M^{-1} \left((K^{\xi})^T Q_k A_k^* + (K^{\eta})^T Q_k B_k^* + (K^{\zeta})^T Q_k C_k^* \right)
$$

Optimisation of Matrix Operations

Apply sparse matrices to multiple DOF-vectors Q_k

$\hat{K}^{\zeta}$ Q_k^n $C_k^\star$ $\hat{K}^{\zeta}$ $\frac{\partial^1}{\partial t^1} Q_k$ $C_k^\star$

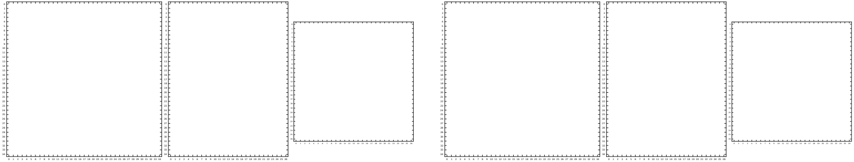


Dense vs. Sparse Kernels: (Breuer et al. [2])

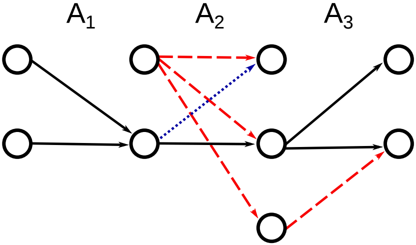
- most kernels fastest, if executed as dense matrix multiplications
- exploit zero-blocks generated during recursive CK computation
- switch to sparse kernels depending on achieved time to solution

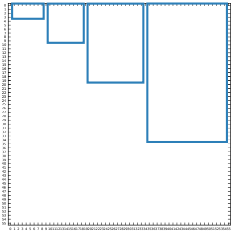
Sparse, Dense → Block-Sparse

Consider equivalent sparsity patterns: (Uphoff, [5])



Graph representation and block-sparse memory layouts





Code Generator: Instrinsics → Assembler

dense_matrices.hpp

dense_matrices.hpp 〉 generatedMatrixMultiplication_dense_56_9_56(double* A, double* B, double* C, double* A_prefetch = NULL, double* B_prefetch = NULL, double* C_prefetch = NULL)

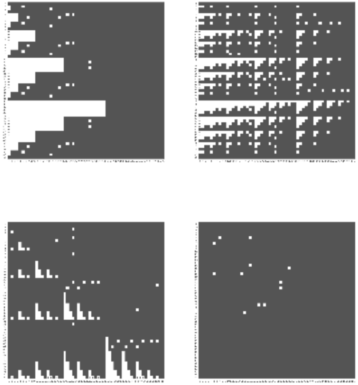
```
inline void generatedMatrixMultiplication_dense_56_9_56(double* A, double* B, double* C, double* A_prefetch = NULL, double* B_prefetch = NULL
        , double* C_prefetch = NULL) {
//[...] SSE and AVX data types, SSE optimization
#if defined(__SSE3__) && defined(__AVX__)
//[...] pointers
for(int n = 0; n < 9; n+=3) {
  for(int m = 0; m < 48; m+=12) {
    //[...] pointers and loads
    for (int k = 0; k < 56; k++)
    {
    b_0 = _mm256_broadcast_sd(b0);
    //[...] more broadcasts and arithmetics on b
    a_0 = _mm256_load_pd(a0);
    a0+=4;
    c_0_0 = _mm256_add_pd(c_0_0, _mm256_mul_pd(a_0, b_0));
    c_0_1 = _mm256_add_pd(c_0_1, _mm256_mul_pd(a_0, b_1));
    c_0_2 = _mm256_add_pd(c_0_2, _mm256_mul_pd(a_0, b_2));
//[...] remaining kernel
#endif

#if defined(__MIC__)
//[...] MIC specifics
for(int n = 0; n < 9; n+=3) {
  //[...] MIC specifics
  #pragma prefetch b0,b1,b2,a0
  for(int k = 0; k < 56; k++)
  {
    //[...] MIC specifics
    c_0_0 = _mm512_fmadd_pd(a_0, b_0, c_0_0);
    c_0_1 = _mm512_fmadd_pd(a_0, b_1, c_0_1);
    c_0_2 = _mm512_fmadd_pd(a_0, b_2, c_0_2);
    a0 += 8;

//[...] remaining MIC kernel
#endif

#if !defined(__SSE3__) && !defined(__AVX__) && !defined(__MIC__)
//[...] fallback code
#endif

#ifndef NDEBUG
num_flops += 56448;
```



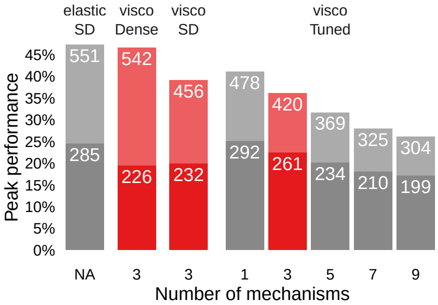
Code Generator – Programming Interface

```
db = Tools.parseMatrixFile('matrices.xml')
Tools.memoryLayoutFromFile('layout.xml', db)
arch = Arch.getArchitectureByIdentifier('dhsw')
volume = db['kXiDivM']
       * db['timeIntegrated']
       * db['AstarT']
       + db['timeIntegrated']
       * db['ET']
kernels = [('volume', volume)]
Tools.generate(
  'path/to/output',
  db,
  kernels,
  'path/to/libxsmm_gemm_generator',
  arch
)
```

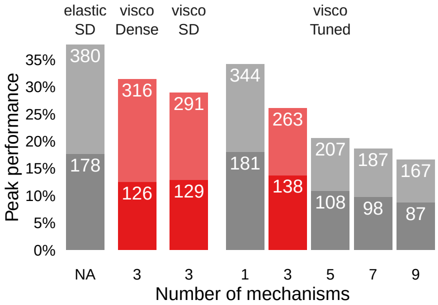
Exploit efficient backend: **libxsmm** library [10]

Floating-Point Performance (Haswell vs. KNC)

Single-node, 65,000 elements, 1000 timesteps, 6-th order



Dual-socket Xeon E5-2697 v3, 28 cores

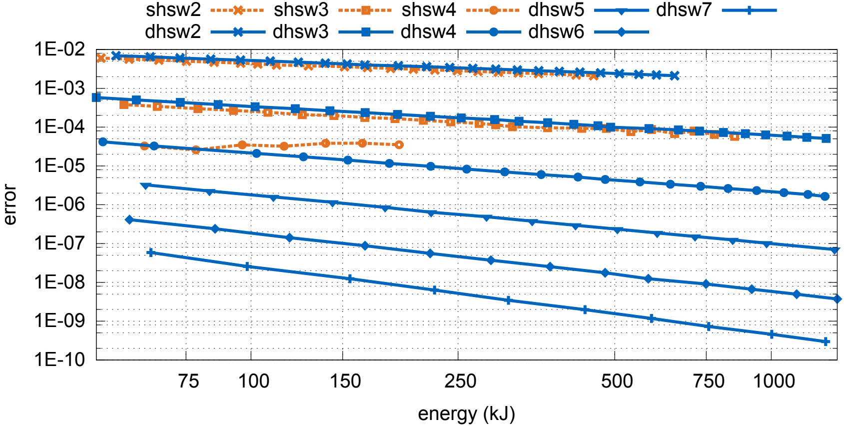


Xeon Phi 5110P, 60 cores

Non-zero flops increase by 13% due to matrix partitioning.

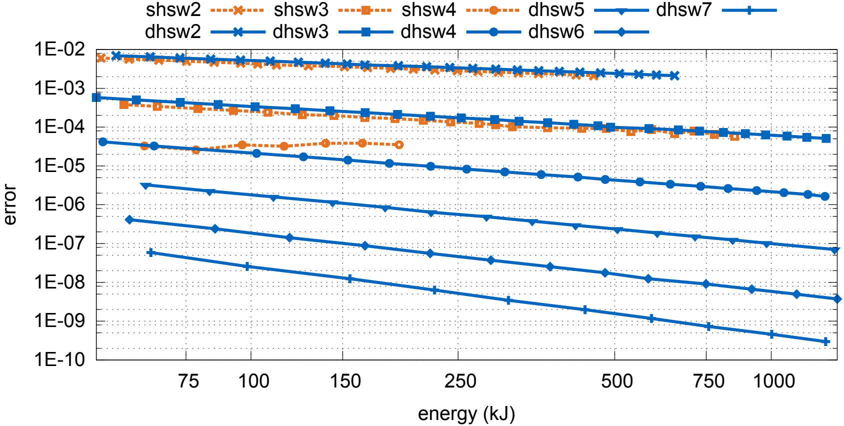
Non-zero flops increase by 7% due to matrix partitioning.

Benefit of High Order ADER-DG – Energy-Efficient



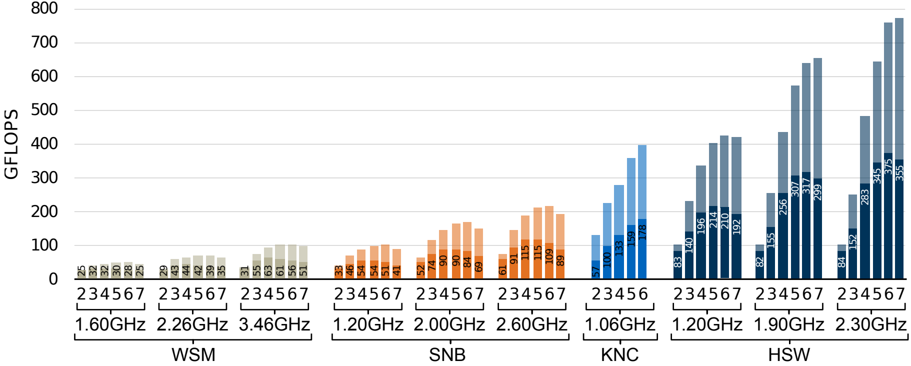
- mesasure maximum error vs. consumed energy
- for increasing discretisation order on regular meshes
- here: dual-socket “Haswell” server, 36 cores @1.9 GHz

Benefit of High Order ADER-DG – Energy-Efficient



- high order (“compute”) beats high resolution (“memory”)
- $\approx$ 35% gain in energy-to-solution for single precision, but only for low order

Benefit of High Order ADER-DG – Compute-Bound



- mesasured “GFlop/s” and “MFlop/s per Watt” for Westmere, Sandy Bridge, Knights Corner and Haswell architectures [1]
- at selected clock frequencies and for different order
- preference towards high order and low frequency on newest architectures

Part III

Accelerators – Dynamic Rupture Simulation on Xeon Phi Supercomputers

Heinecke, Breuer, Rettenberger, Gabriel, Pelties et al. [3]:
Petascale High Order Dynamic Rupture Earthquake Simulations on Heterogeneous Supercomputers (Gordon Bell Prize Finalist 2014)

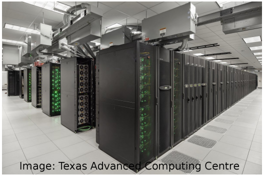
On the Road from Peta- to Exascale?

SuperMUC @ LRZ, Munich

- 9216 compute nodes (18 “thin node” islands)
  147,456 Intel SNB-EP cores (2.7 GHz)
- Infiniband FDR10 interconnect (fat tree)
- #20 in Top 500: 2.897 PFlop/s

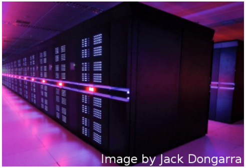
Stampede @ TACC, Austin

- 6400 compute nodes, 522,080 cores
  2 SNB-EP (8c) + 1 Xeon Phi SE10P per node
- Mellanox FDR 56 interconnect (fat tree)
- #8 in Top 500: 5.168 PFlop/s



Tianhe-2 @ NSCC, Guangzhou

- 8000 compute nodes used, 1.6 Mio cores
  2 IVB-EP (12c) + 3 Xeon Phi 31S1P per node
- TH2-Express custom interconnect
- #1 in Top 500: 33.862 PFlop/s



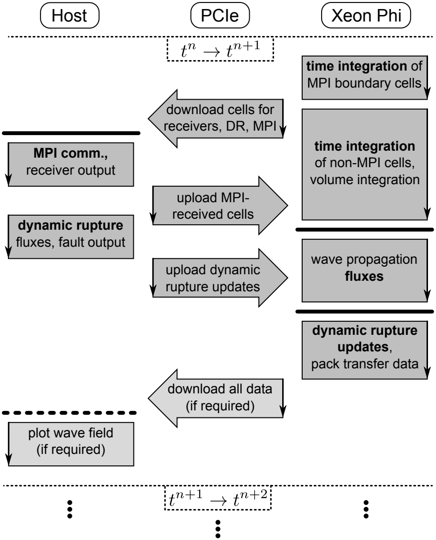
Optimization for Intel Xeon Phi Platforms

Offload Scheme:

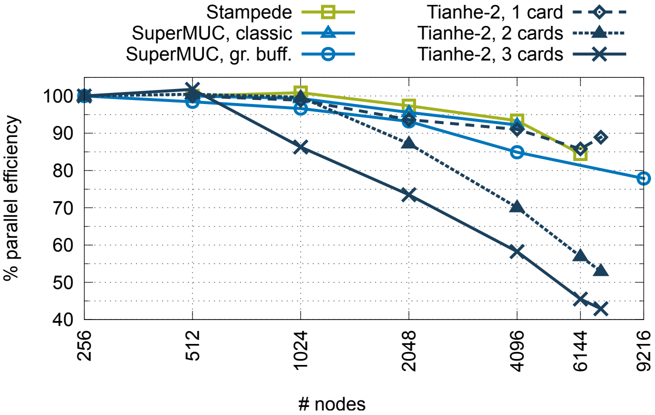
- hide2 communication with Xeon Phi and between nodes
- use “heavy” CPU cores for dynamic rupture

Hybrid parallelism:

- on 1–3 Xeon Phis and host CPU(s)
- reflects multiphysics simulation
- manycore parallelism on Xeon Phi

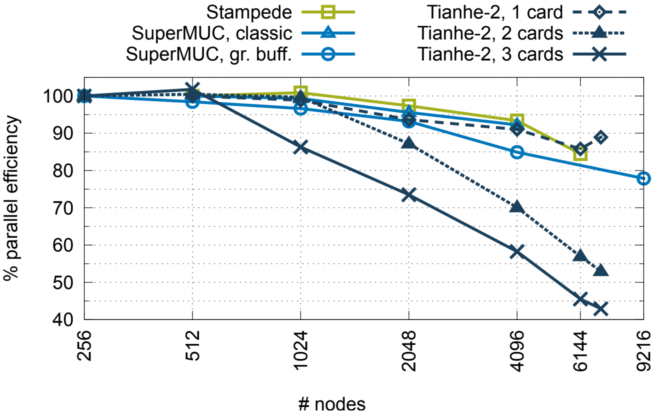


Strong Scaling of Landers Scenario



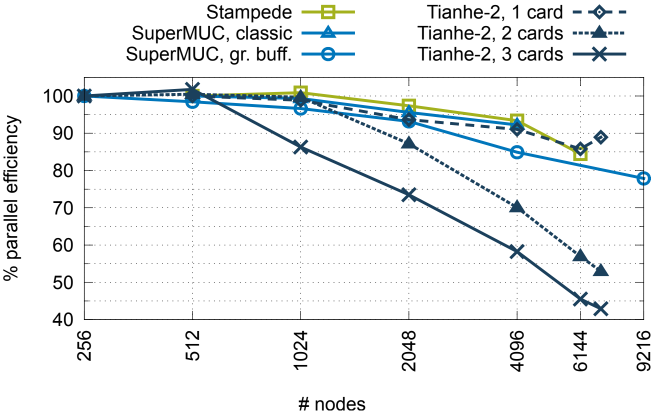
- 191 million tetrahedrons; 220,982 element faces on fault
- 6th order, 96 billion degrees of freedom

Strong Scaling of Landers Scenario



- more than 85 % parallel efficiency on Stampede and Tianhe-2 (when using only one Xeon Phi per node)
- multiple-Xeon-Phi performance suffers from MPI communication

Strong Scaling of Landers Scenario



- 3.3 PFlop/s on Tianhe-2 (7000 nodes)
- 2.0 PFlop/s on Stampede (6144 nodes)
- 1.3 PFlop/s on SuperMUC (9216 nodes)

Optimizing SeisSol for Xeon Phi (Knights Landing)

Heinecke, Breuer et al., ISC 16 [7]

Code Generation:

- 512-bit wide vector processing unit
- profits from Knights Landing optimization of libxsmm library [10]

Memory Optimization:

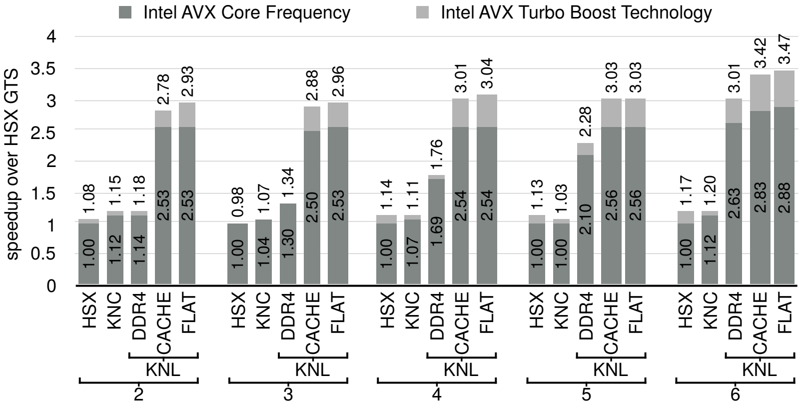
- examine impact of DRAM-only, CACHE and FLAT mode
- FLAT mode: careful placement of element-local matrices in local MCDRAM (table from [7]):

order	Q_k	$\mathcal{B}_k, \mathcal{D}_k$	$A_k^{\xi_c}, \hat{A}_k^{-,i}, \hat{A}_k^{+,i}$	$\hat{K}^{\xi_c}, \tilde{K}^{\xi_c}, \hat{F}^{-,i}, \hat{F}^{+,i,j,h}$
2	MCDRAM	MCDRAM	MCDRAM	MCDRAM
3	MCDRAM	MCDRAM	MCDRAM	MCDRAM
4	DDR4	MCDRAM	MCDRAM	MCDRAM
5	DDR4	MCDRAM	DDR4	MCDRAM
6	DDR4	MCDRAM	DDR4	MCDRAM

$\rightarrow$ see “KNL Book” [8] for details

Performance Results on Knights Landing

Heinecke et al., ISC 16 [7]



Landers scenario, 466,574 elements

Part IV

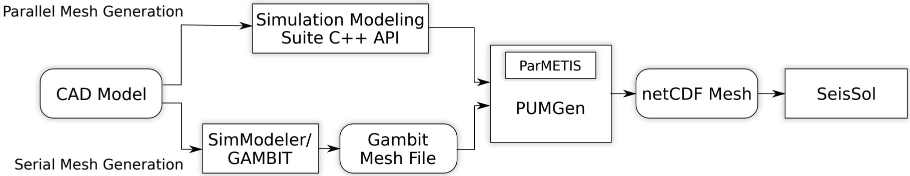
Current Work – Simulations in Symmetric Mode on Salomon

Salomon: 2 PFlop/s supercomputer (432 nodes with 2 HSW + 2 KNC)
at IT4Innovations supercomputing centre, Ostrava

Rettenberger, Uphoff, Rannabauer;
Project CzeBaCCA: Czech-Bavarian Competence Centre for Supercomputing Applications

Modify Mesh Input and Load Distribution

Scalable Mesh Partitioning and Input Pipeline:

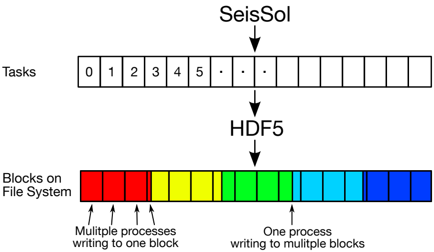


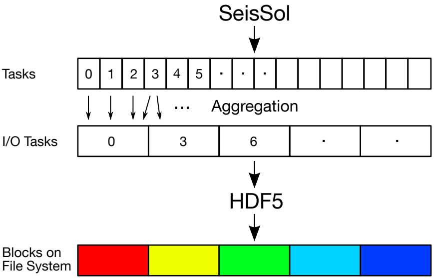
Towards Symmetric Mode:

- Modify weights for METIS graph partitioning:
  compensate speed differences between host CPU and Xeon Phi
- Work in progress: modify input of meshes
  → Xeon Phi mesh partitions may be read by host and sent via MPI
  → in case of bad I/O bandwidth (library support) of Xeon Phis

Work in Progress: Modify Wave Field Output

Aggregation of MPI ranks to speed up I/O: (Rettenberger [4])



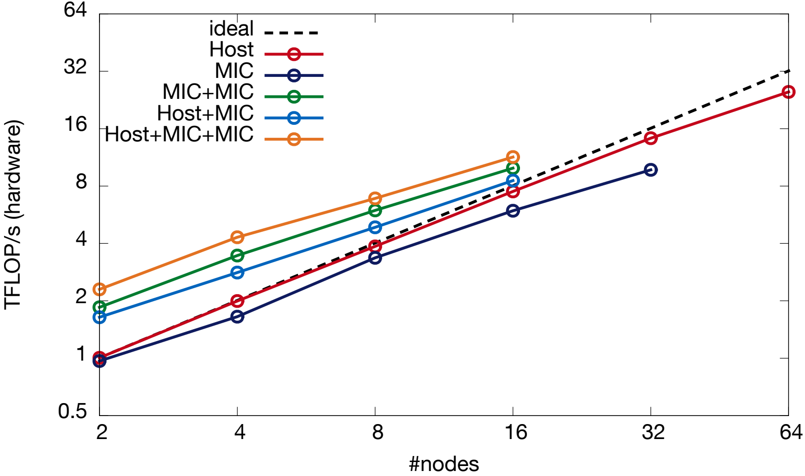


Towards Symmetric Mode:

- Output routines aggregate data from several MPI ranks
  $\rightarrow$ match I/O block size to achieve substantial speedup
- Only use host MPI ranks for output
  $\rightarrow$ again in case of bad I/O bandwidth (library support) of Xeon Phis

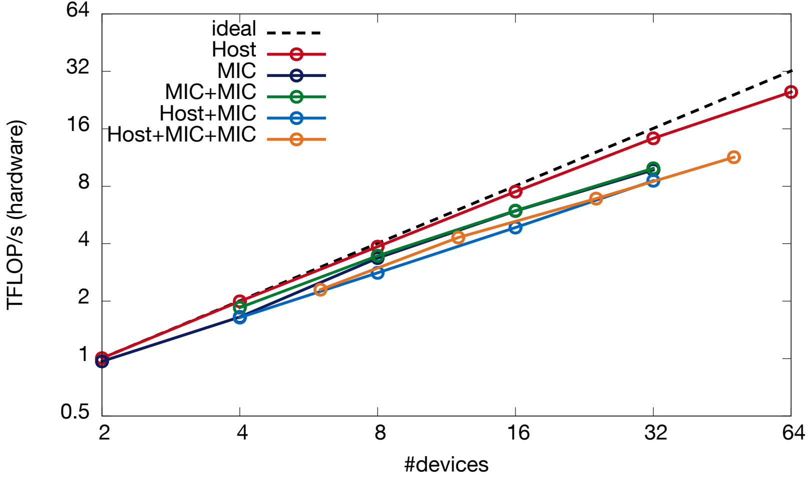
First Runs on Salomon – Native and Symmetric

Setup: LOH4 benchmark, 250k elements, order 6, no output yet



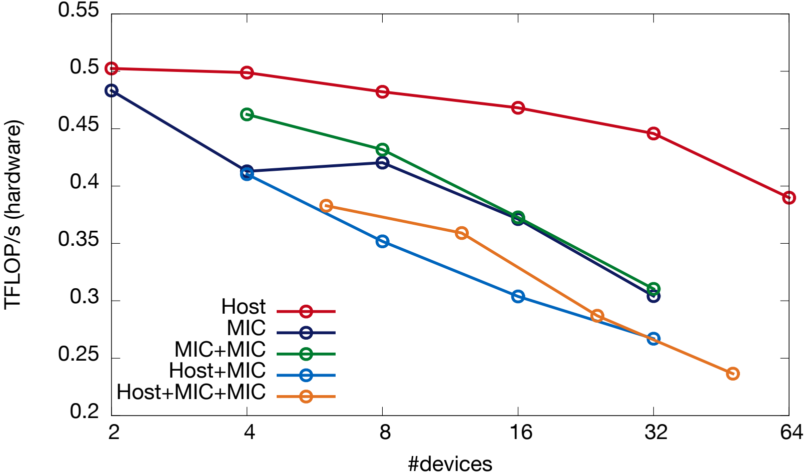
First Runs on Salomon – Native and Symmetric

Setup: LOH4 benchmark, 250k elements, order 6, no output yet



First Runs on Salomon – Native and Symmetric

Setup: LOH4 benchmark, 250k elements, order 6, no output yet



Part V

Conclusions and Outlook

Conclusions

Performance Optimisation on Multi&Manycore Platforms:

- high convergence order and high computational intensity of ADER-DG
  $\rightarrow$ compute-bound performance on current and imminent CPUs
- code generation to accelerate element kernels
- careful tuning and parallelisation of the entire simulation pipeline
  (scalable mesh input, output and checkpointing)

Xeon Phi Platforms

- offload scheme scaled to 1.5 million cores (Tianhe-2, Stampede)
- our assumption: heterogeneity will prevail; off-loading not necessarily
- our goal: scale in symmetric mode on KNC-based supercomputers
  $\rightarrow$ current work on SuperMIC and esp. Salomon
- heterogeneity challenges exist in load balancing and scalable I/O
- SeisSol runs on Knights Landing $\rightarrow$ ISC'16 [7] and KNL-Book [8]

Acknowledgements

Special thanks go to ...

- the entire SeisSol team and all contributors, esp.:
  - Alex Breuer, Sebastian Rettenberger, Carsten Uphoff
  - Alex Heinecke
  - Alice Gabriel, Christian Pelties, Stephanie Wolherr
- all colleagues from the Leibniz Supercomputing Centre
- all colleagues from the IT4Innovations Supercomputing Centre
- for financial and project support:
  - Intel Corporation (IPCC ExScaMIC)
  - Volkswagen Foundation (project ASCETE)
  - BMBF (project CzeBACCA)

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