DM-HEOM:
A Portable and Scalable Solver-Framework for the Hierarchical Equations of Motion

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Tobias Kramer, Thomas Steinke

Zuse Institute Berlin
Distributed Algorithms and Supercomputing

Motivation

Observations:

- many HPC applications are **legacy code**
  - $\Rightarrow$ written and incrementally improved **by domain scientists**
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What can we do better? – Our Suggestion:

- **portability first**, then portable performance
- **interdisciplinary collaborations** where computer scientists design the software
- **modern methods and technologies** with a community beyond HPC

Contributions

a) 1st **D**istributed **M**emory implementation of the **HEOM** method: **DM-HEOM**

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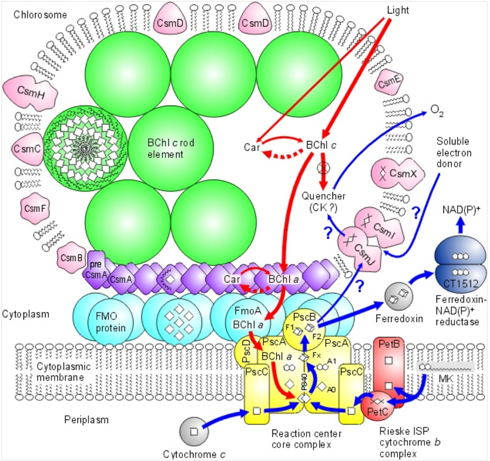
c) Design guidelines/experiences for **performance portable** HPC applications

HEOM - Hierarchical Equations of Motion

Model for Open Quantum Systems

- understand the energy transfer in photo-active molecular complexes
  - ⇒ e.g. **photosynthesis**

  ... but also **quantum computing**



[Image by University of Copenhagen Biology Department]

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$$\begin{aligned}
\frac{d\sigma_u}{dt} &= -\frac{i}{\hbar}[H, \sigma_u] \\
&- \sigma_u \sum_{b=1}^{B} \sum_{k}^{K-1} n_{u,(b,k)} \gamma(b,k) \\
&- \sum_{b=1}^{B} \left[\frac{2\lambda_b}{\beta \hbar^2 \nu_b} - \sum_{k}^{K-1} \frac{c(b,k)}{\hbar \gamma(b,k)} \right] V_{s(b)}^{\times} V_{s(b)}^{\times} \sigma_u \\
&+ \sum_{b=1}^{B} \sum_{k}^{K-1} i V_{s(b)}^{\times} \sigma_{u,b,k}^{+} \\
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- hierarchical graph of complex matrices (auxiliary density operators, ADOs)
  - ⇒ dim: $N_{\text{sites}} \times N_{\text{sites}}$
  - ⇒ count: **exp. in hierarchy depth** d

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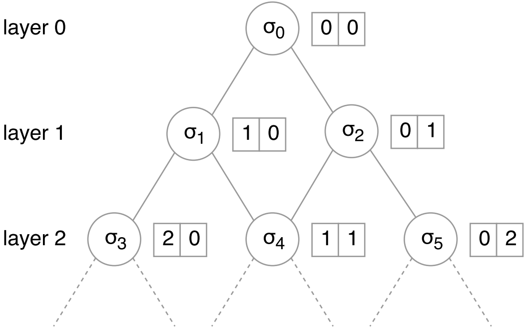

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Device Name (architecture)	compute [TFLOPS]	memory bw. [GiB/s]	[FLOP/Byte]
2× Intel Xeon Gold 6138 (SKL)	2.56	238	**10.8**
2× Intel Xeon E5-2680v3 (HSW)	0.96	136	**7.1**
Intel Xeon Phi 7250 (KNL)	2.61[a]	490/115[b]	**5.3/22.7**[b]
Nvidia Tesla K40 (Kepler)	1.31	480	**2.7**
AMD Firepro W8100 (Hawaii)	2.1	320	**6.6**

[a] Assuming 1.2 GHz AVX frequency. [b] On-chip MCDRAM / DRAM

HEOM - Example Systems

system name	N_{sites}	**baths per site**	**depth** d	**total ADO memory**
FMO	7	22	8	2.8 GiB
LHC II monomer	14	1	3	5.6 GiB
PS I	**96**	1	**3**	**129.2 GiB**
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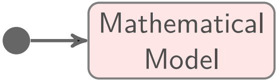
⇒ distributed memory implementation **required**

Interdisciplinary Workflow

domain experts computer scientists



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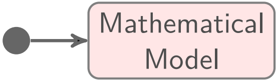

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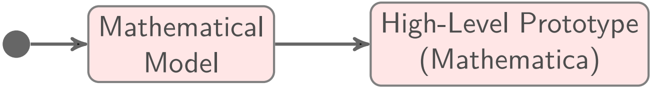

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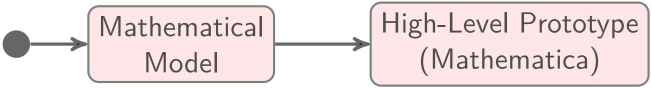

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- symbolic solvers
- arbitrary precision
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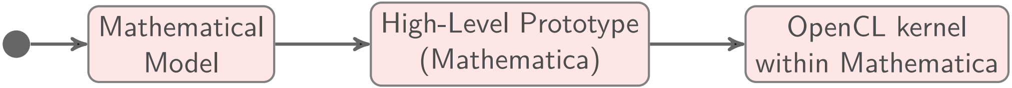

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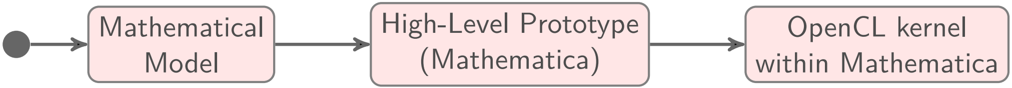

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OpenCL (Open Computing Language) in a Nutshell

- open, royalty-free **standard** for cross-platform, **parallel programming**
- maintained by **Khronos Group**
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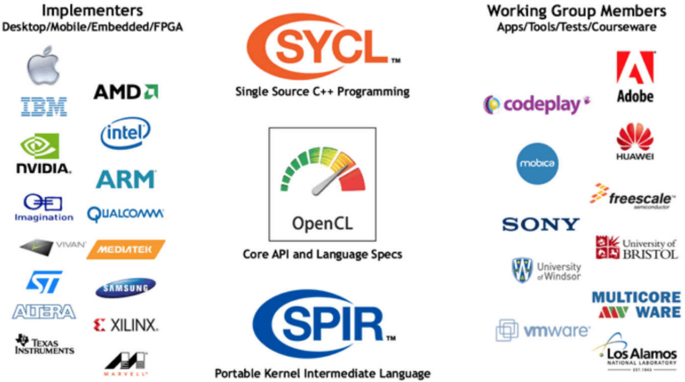
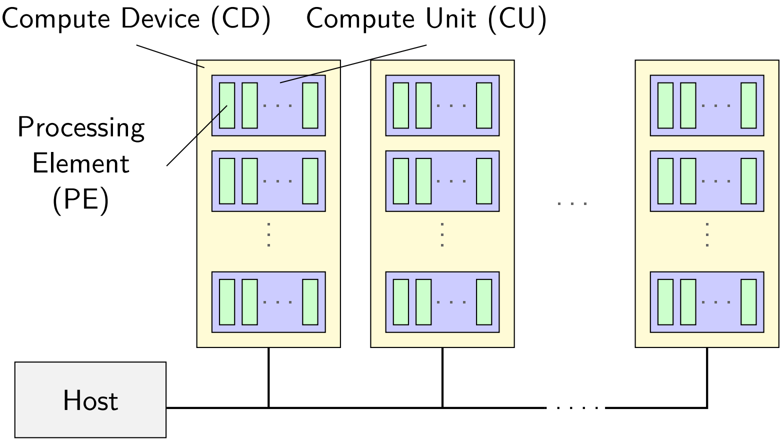


OpenCL Platform and Memory Model



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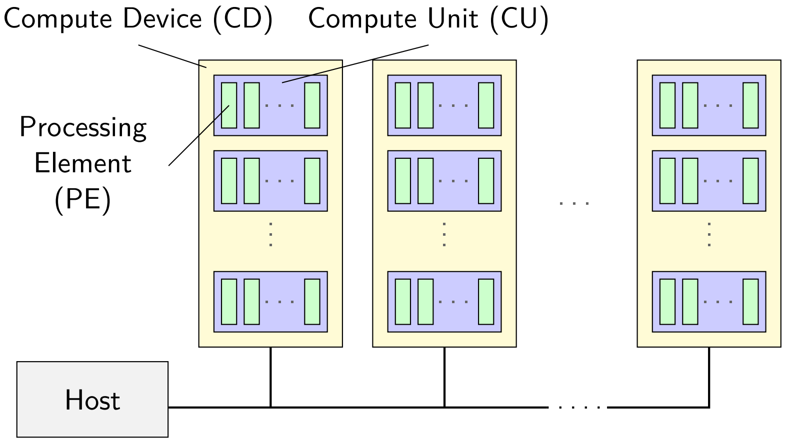

Memory Model:

- CD has device memory with **glottal/constant** addr. space
- CU has **local** memory addr. space
- PE has **private** memory addr. space

⇒ relaxed consistency

OpenCL Machine Model Mapping

OpenCL Platform	CPU Hardware	GPU Hardware
Compute Device	Processor/Board	GPU device
Compute Unit	Core (thread)	Streaming MP
Processing Element	SIMD Lane	CUDA Core
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- ⇒ currently: **widest practical portability** of parallel programming models

Interdisciplinary Workflow

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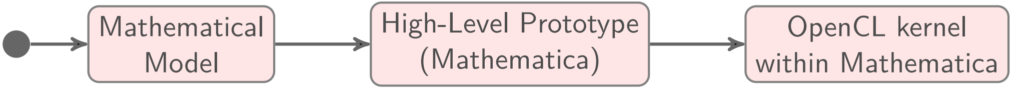

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- ODEs
- PDEs
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- ...

High-Level Prototype (Mathematica):
- domain scientist's tool
- high level
- symbolic solvers
- arbitrary precision
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OpenCL kernel within Mathematica:
- replace some code with OpenCL
- compare results
- figure out numerics
- use accelerators in MM

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- **separation and exchangeability** of different aspects and strategies
  - partitioning, numerical methods, memory layout, parallelisation, communication, etc.

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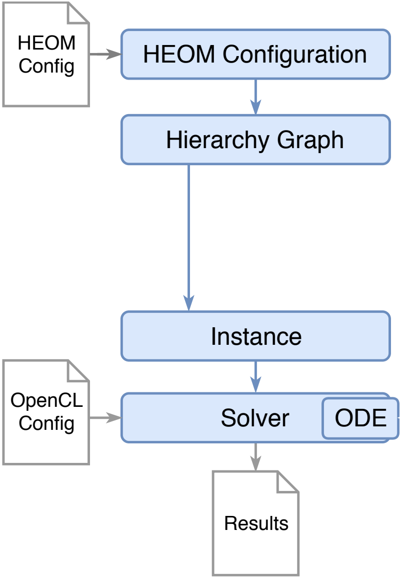
- start single node
- OpenCL 1.2 for hotspots
- modern C++ 11/14/17
- CMake for building

Distributed Memory HEOM: Single Node C++ Application



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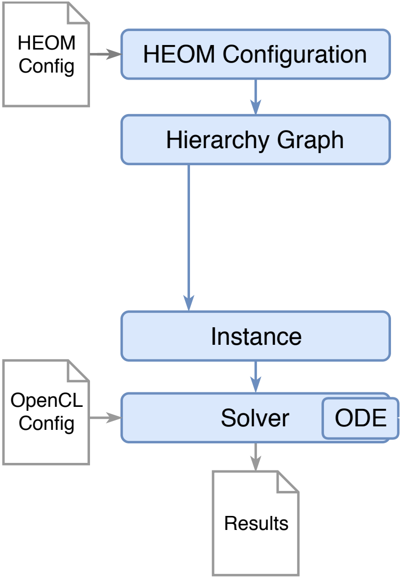

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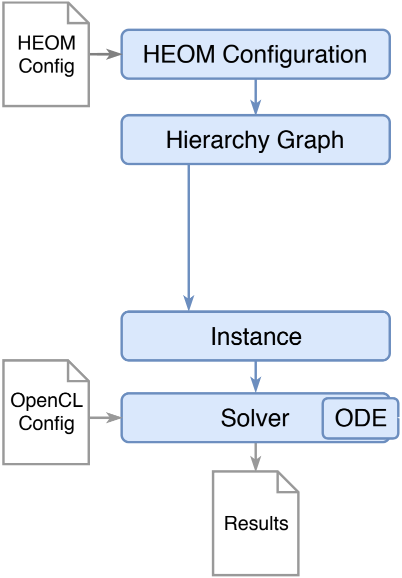

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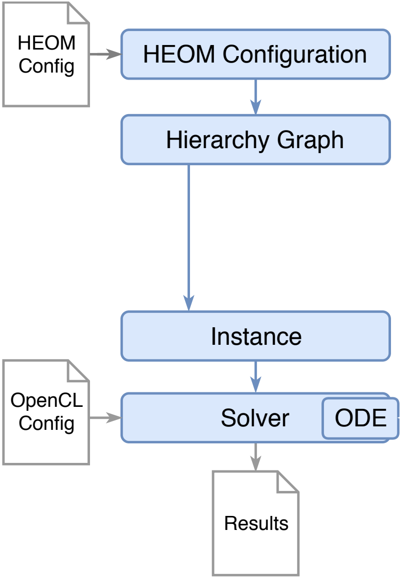

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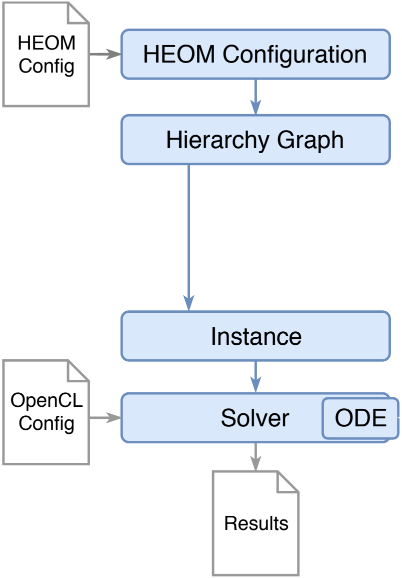

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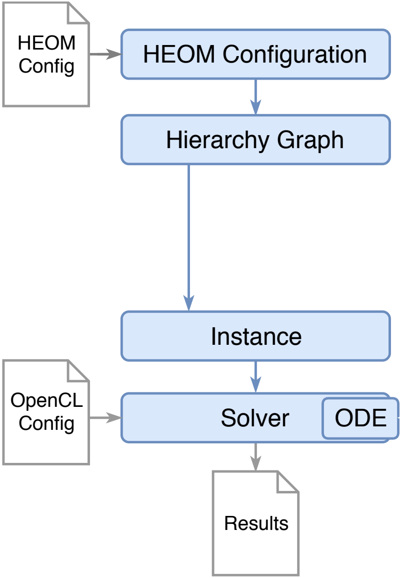

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- *OpenCL Config* specifies runtime configuration
- *Solver* works on *ODE*
  - ⇒ encapsulates OpenCL runtime
  - ⇒ encapsulates numerics
  - ⇒ produces *Results*

From Portability to Performance

OpenCL:

- guarantees portability ...
- ... but no portable performance

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Strategy:

1. identify key optimisations each device requires
2. make the code configurable to the device's needs

   ... without writing a version for each device

Performance Portability: Node-Level

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b) configurable kernel code:

- work-item granularity
- memory-layout

Performance Portability: Work-item Granularity

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- processed on the smallest parallel hardware execution unit (PE)

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⇒ requires a **compile-time configurable outer loop-nest** inside the kernel

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⇒ match requirement of **device-specific memory architecture**

- **GPU**: coalesced access from working-groups without bank-conflicts
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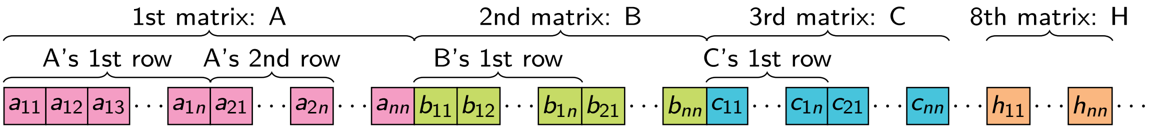
⇒ **parallelisation strategy**, **granularity** and **memory layout** must match

- e.g. outer loop vectorisation for SIMD architectures

AoS vs. SIMD-friendly AoSoA Memory Layout



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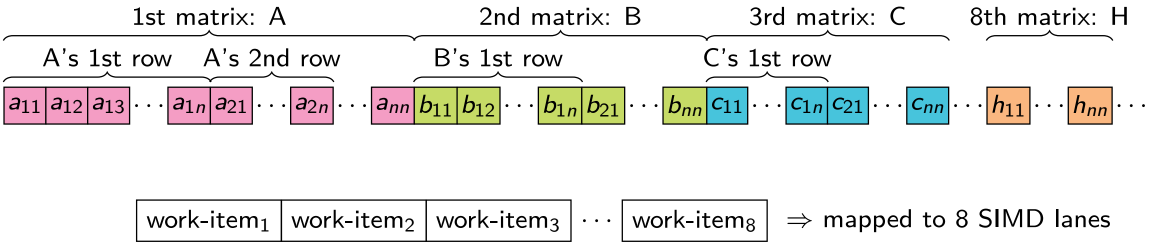

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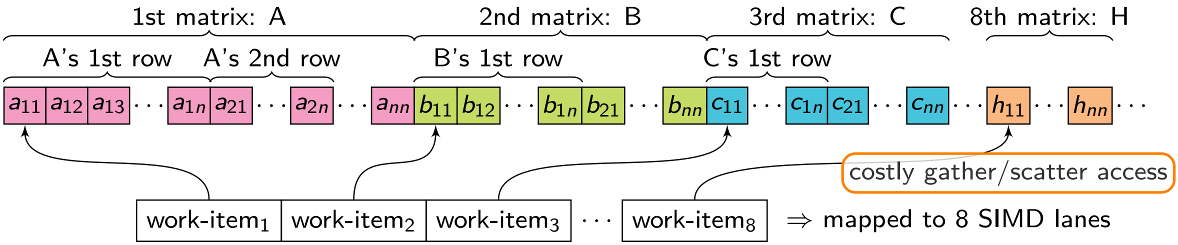

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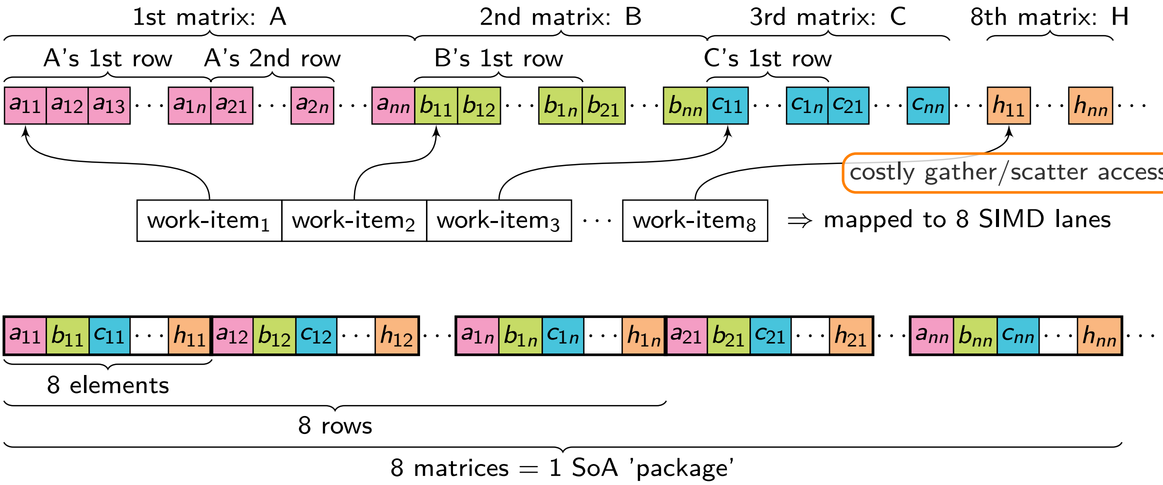

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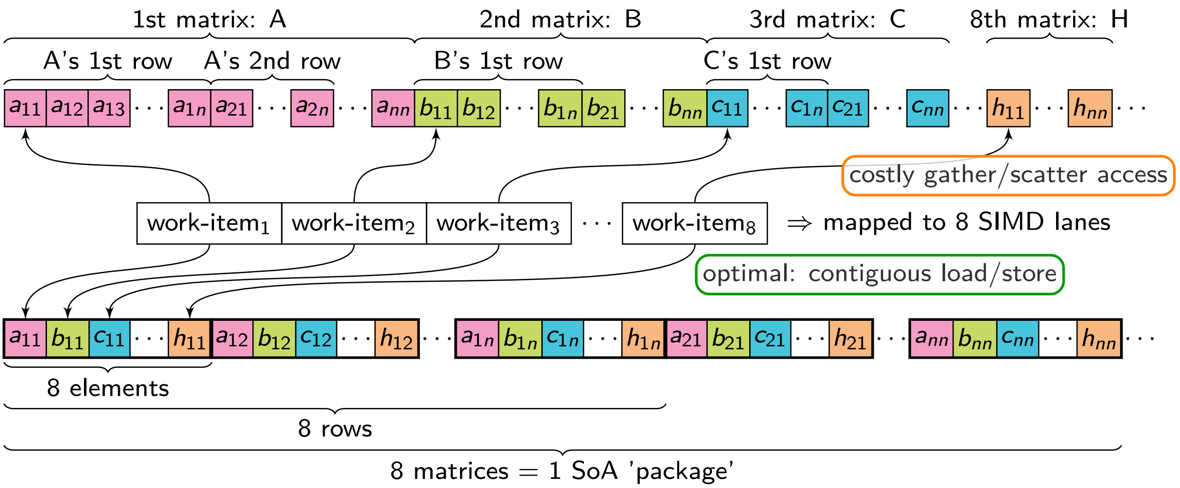

Interdisciplinary Workflow

domain experts | computer scientists

Mathematical Model → **High-Level Prototype (Mathematica)** → **OpenCL kernel within Mathematica** → . . .

Mathematical Model

- ODEs
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- Graphs
- . . .

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- high level
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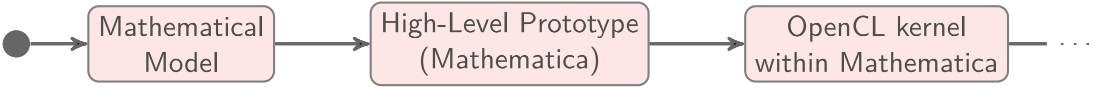

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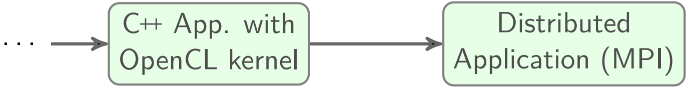

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- **Problem**: map hierarchy graph nodes to n partitions (compute nodes)
  - minimise communication
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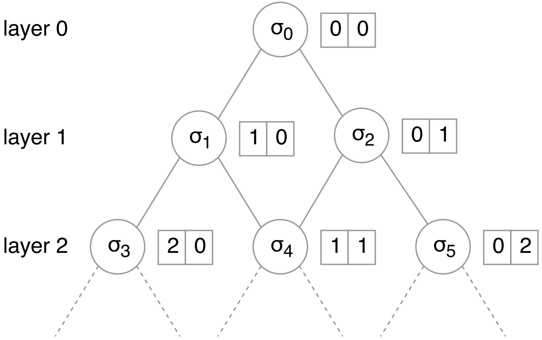

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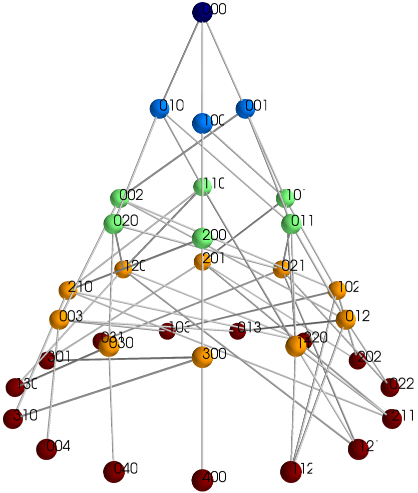

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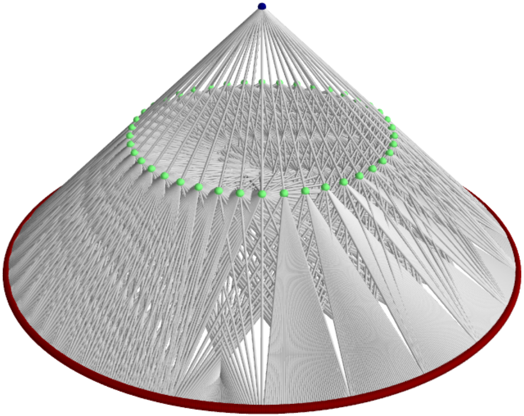

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  - partitioning quality mostly resilient to METIS settings

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64	62	60	63	2451	96.8 %	4739	193.2 %
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$\Rightarrow$ highly connected partitioning graph
$\Rightarrow$ almost **all-to-all**

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$\Rightarrow$ almost all nodes required by other partitions
$\Rightarrow$ prevents inner/outer communication/computation overlap

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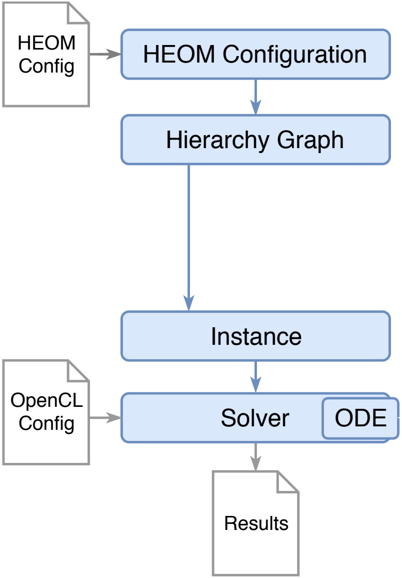
$\Rightarrow$ more halo nodes than local nodes

Distributed Memory HEOM: Multi-Node C++ Application



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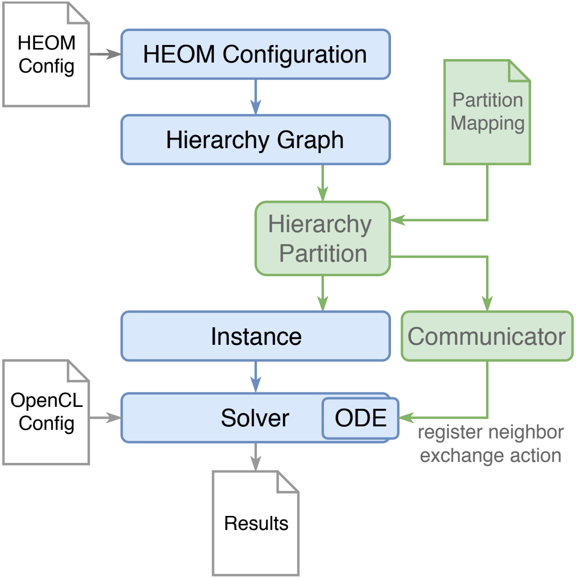

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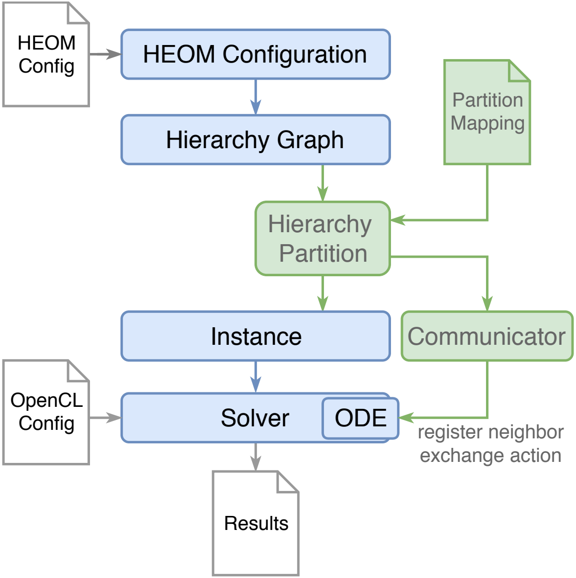

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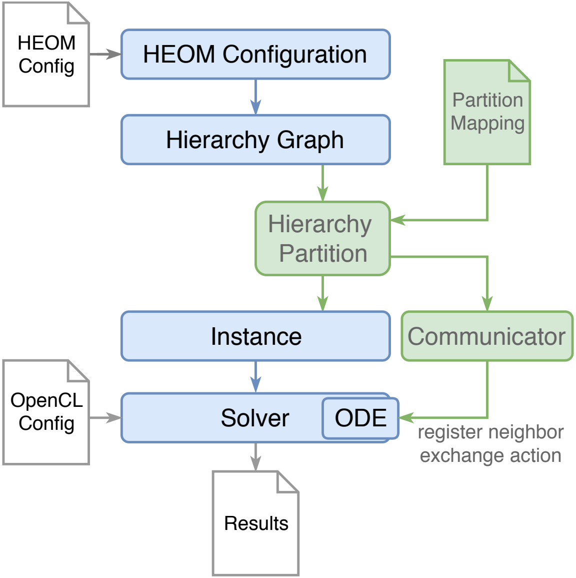

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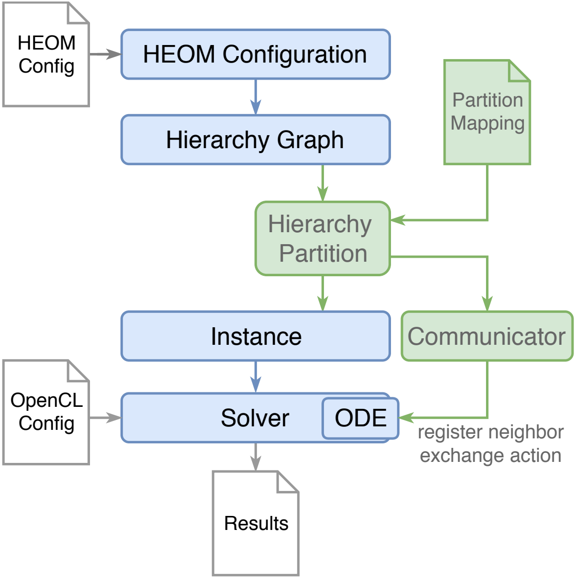

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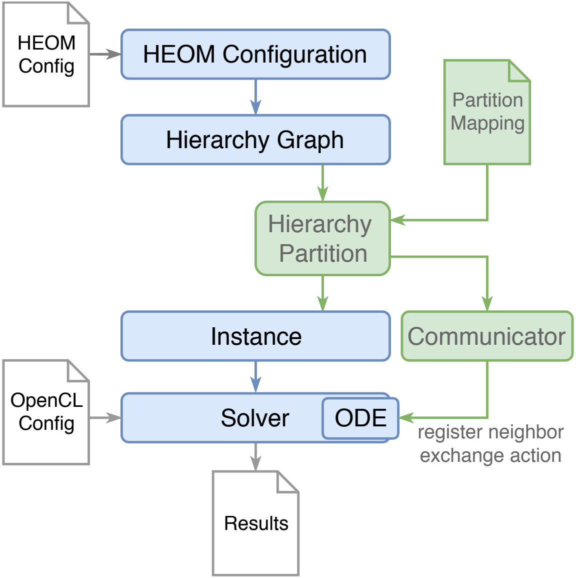

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  - ⇒ fully **declarative** communication API
- *ODE* can trigger action
  - ⇒ neighbor exchange prior to evaluation

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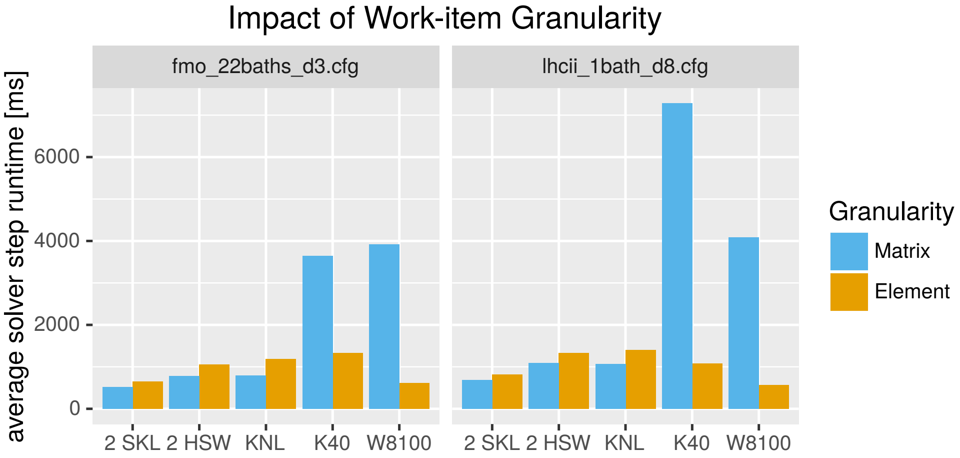
Optimisation / Production Runs
- always collect perf. data
- profile/tune code
- explore new architectures

Benchmarks: Work-item Granularity



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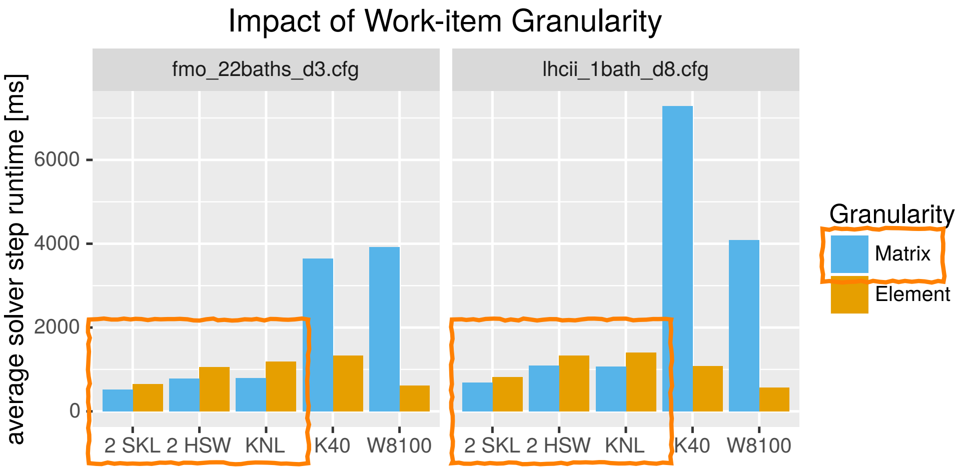

⇒ **CPUs**: 1.2× to 1.35× speedup for Matrix granularity

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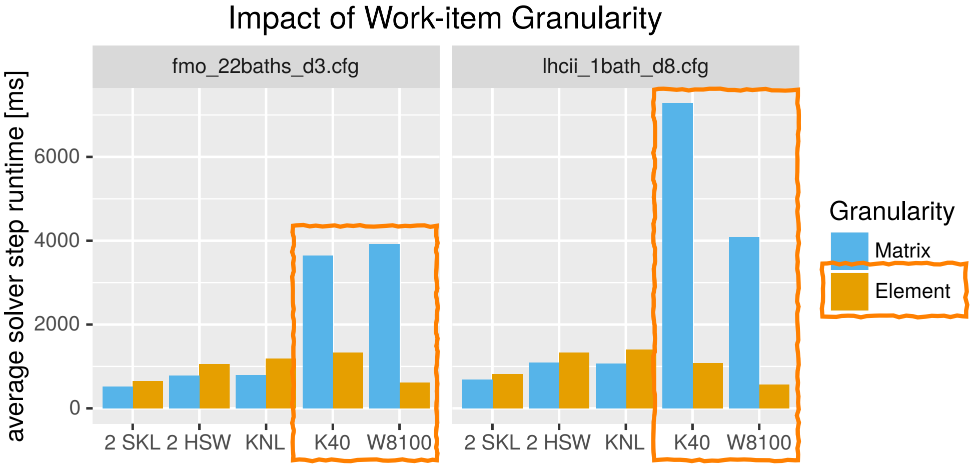
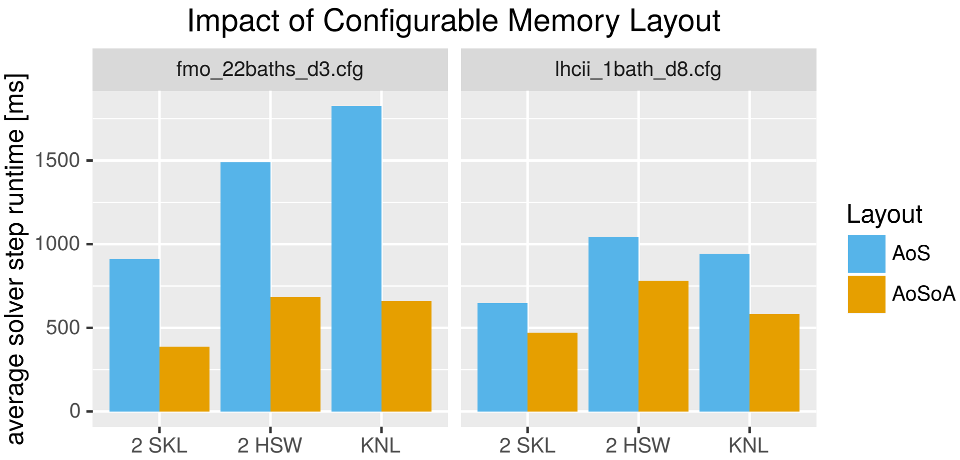


⇒ **GPUs**: up to 6.7× (K40) and 7.2× (W8100) speedup for Element granularity

Benchmarks: Memory Layout



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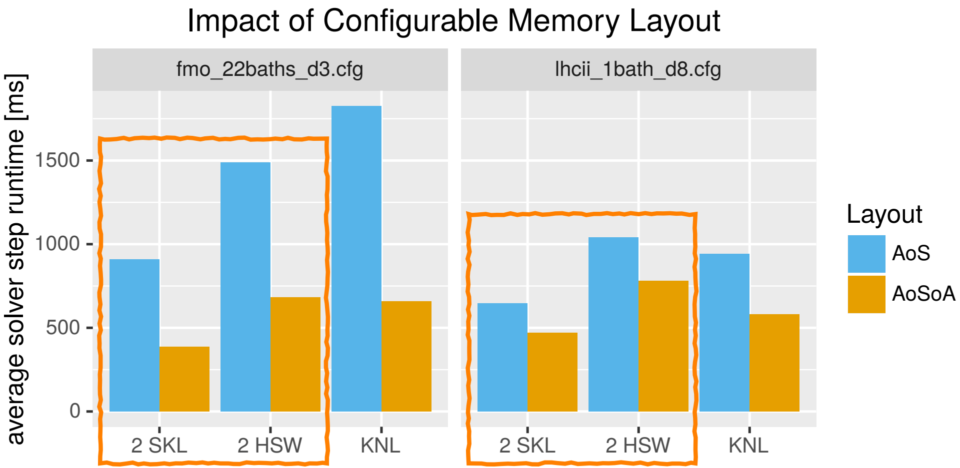

⇒ **SKL** and **HSW**: 1.3× to 2.4× speedup with AoSoA

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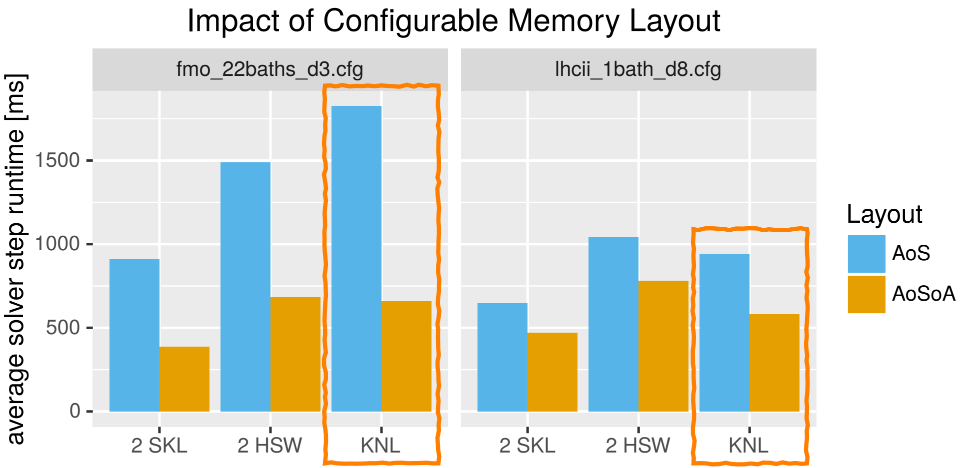
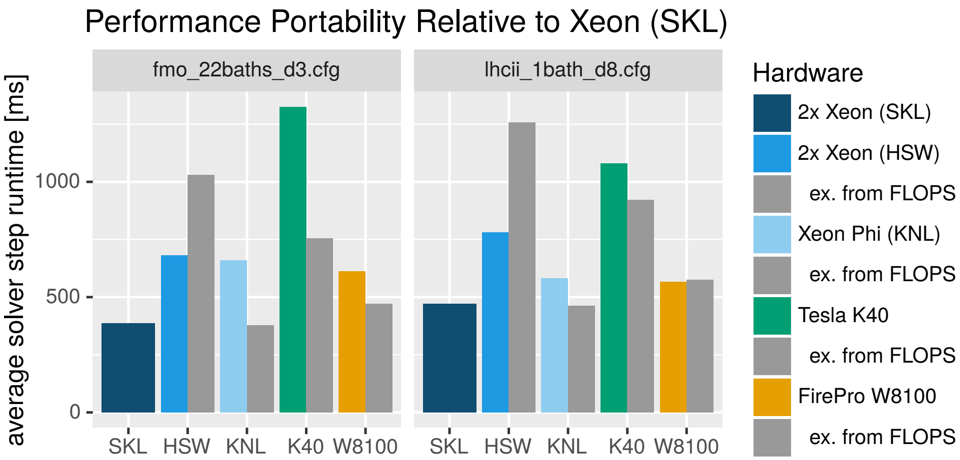


⇒ **KNL**: 1.6× to 2.8× speedup with AoSoA

Benchmarks: Performance Portability



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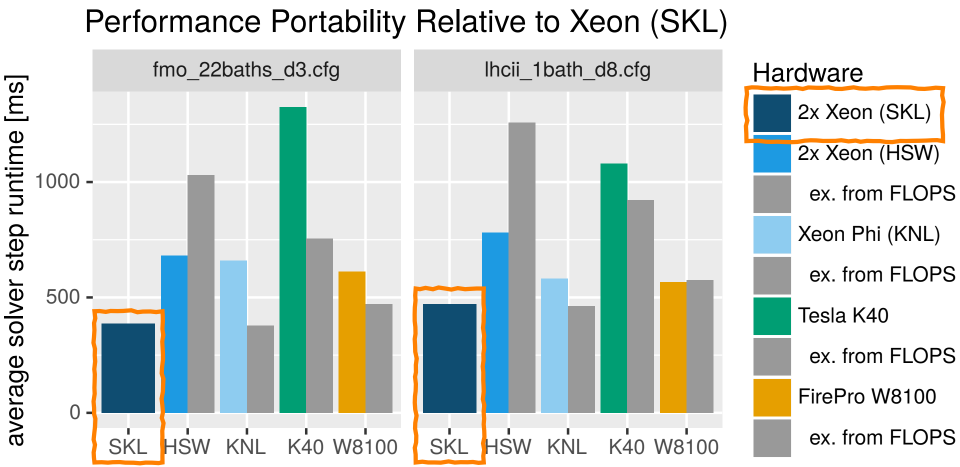

⇒ **SKL** (Xeon) is the **reference**

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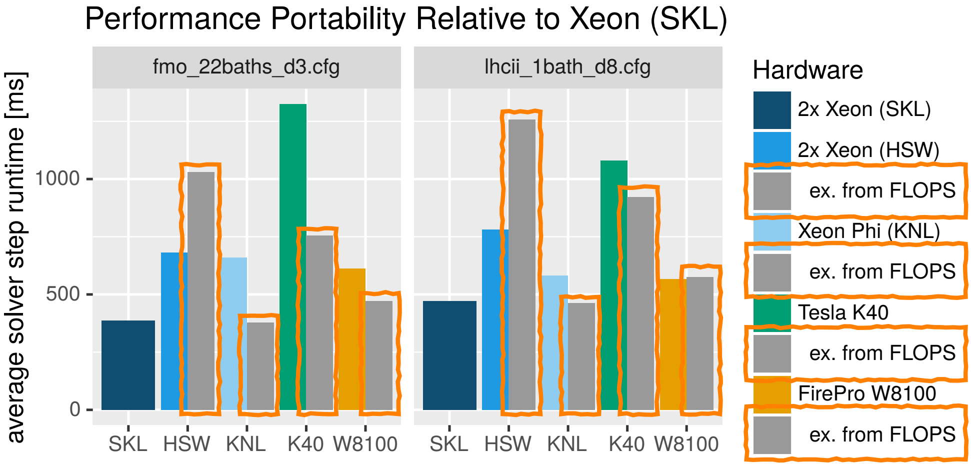

⇒ gray bars are **expected runtimes** extrapolated from peak FLOPS

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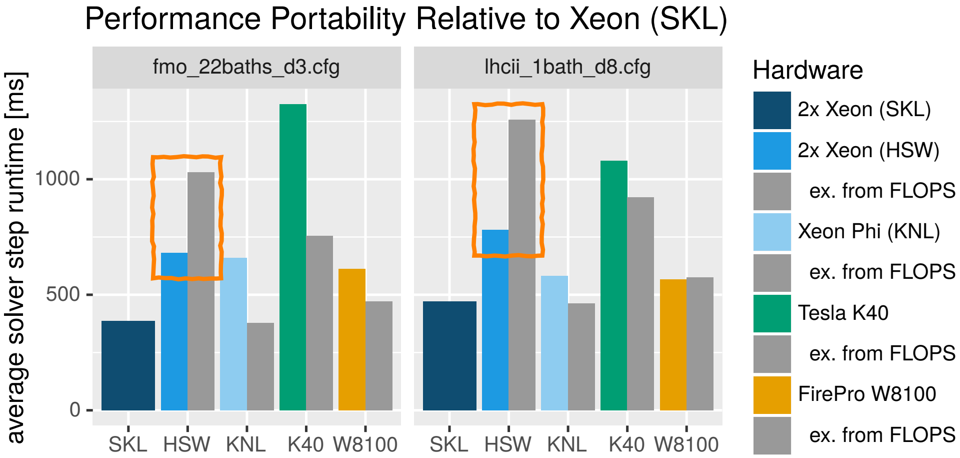

⇒ Older Haswell Xeon exceeds expectations, due to better OpenCL support

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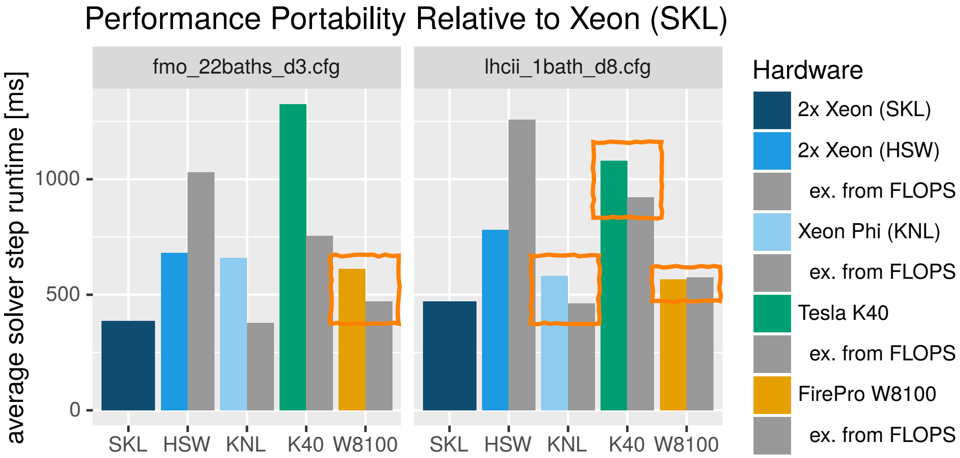

⇒ Good: within 30 % of expectation

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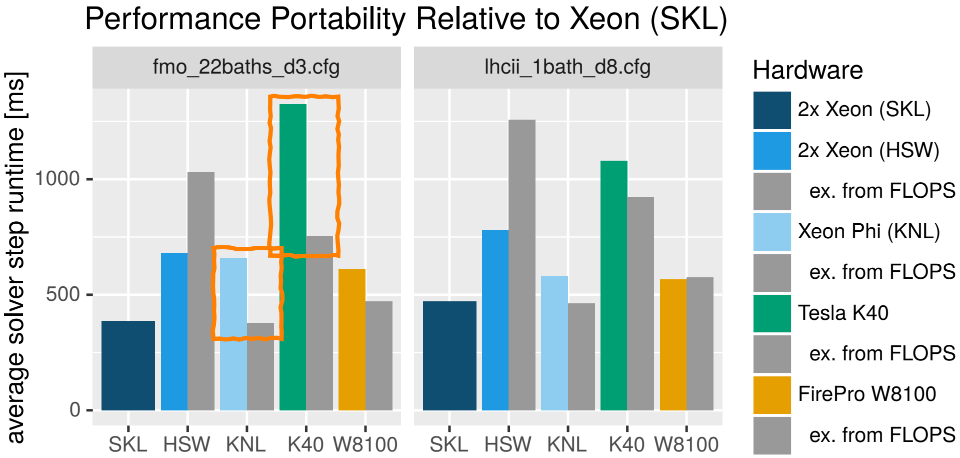

⇒ KNL and K40 sensitive to **irregular accesses** from extreme coupling in this scenario.

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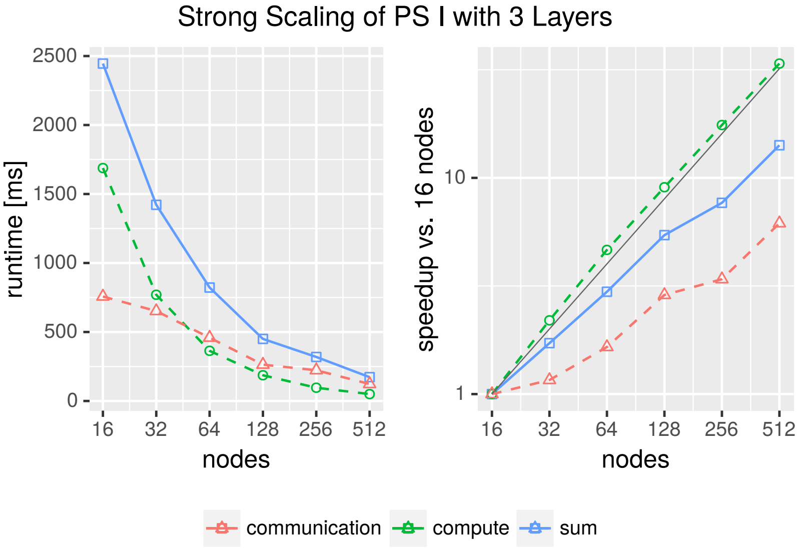

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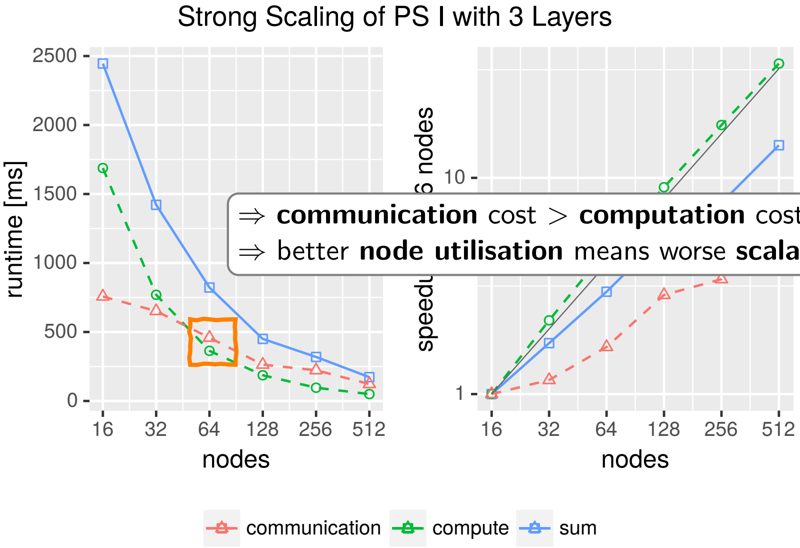

⇒ **communication** cost > **computation** cost

⇒ better **node utilisation** means worse **scalability**

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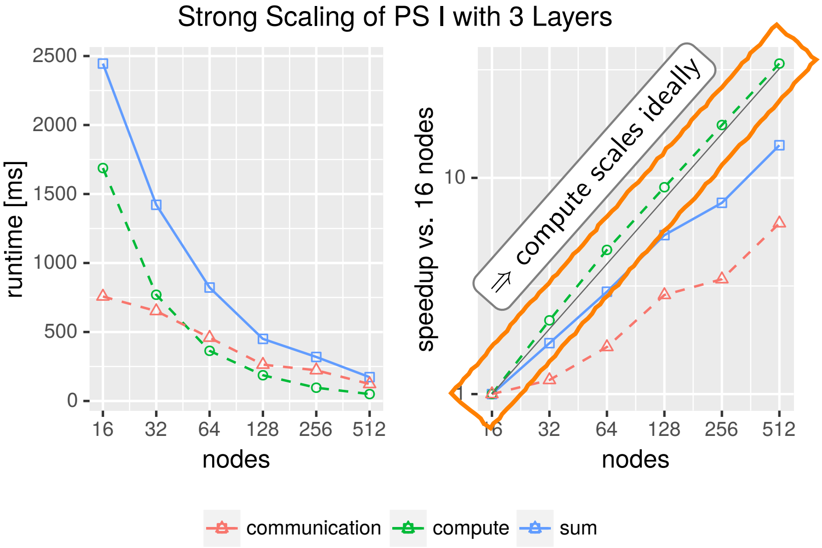

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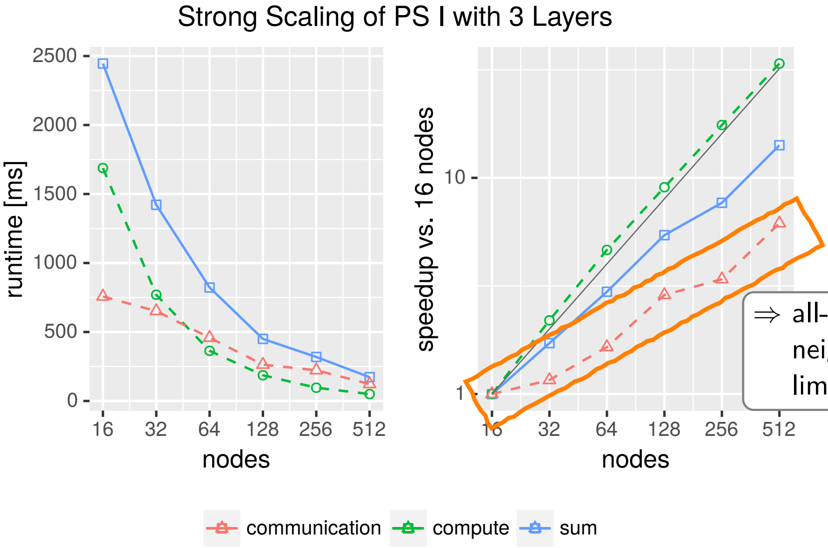

⇒ all-to-all like neighbour-exch. limits scalability

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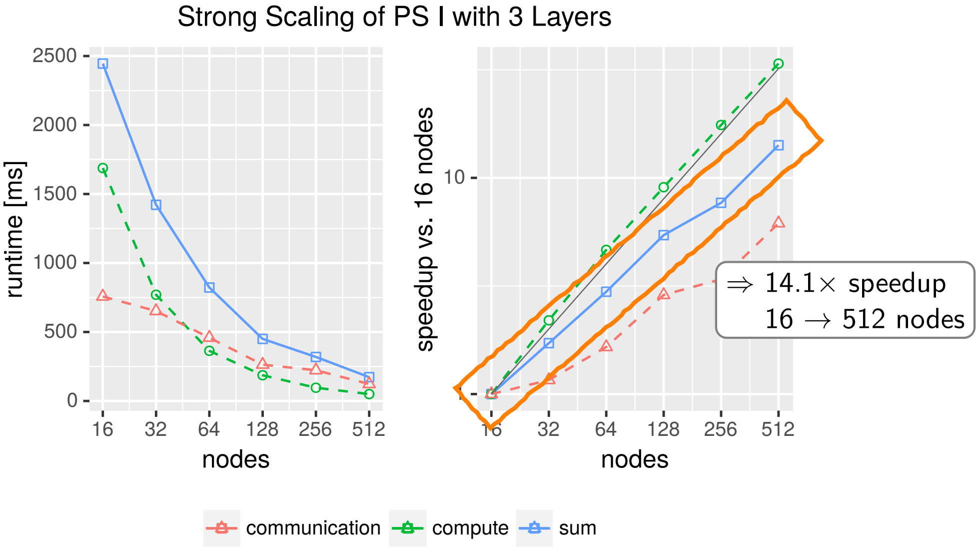

Summary

Lessons's learned:

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- standards (OpenCL, MPI-*3*, . . .) enable **portability**
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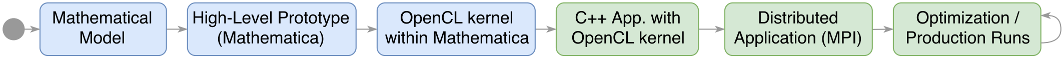
  - ⇒ leverage **runtime compilation**
  - ⇒ **work-item granularity** and **memory and layout**



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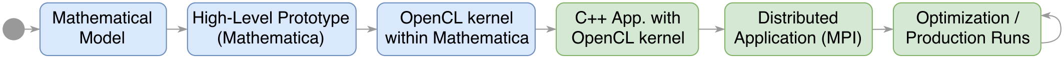

DM-HEOM:

- first **Distributed Memory HEOM** implementation
- pushes the boundary of **feasible problem sizes**
- **practical scalability** from laptops to supercomputers

Thank you.

Feedback? Questions? Ideas?

noack@zib.de

This work was funded by the Deutsche Forschungsgemeinschaft (DFG), projects RE 1389/8-1 and KR 2889/7-1. Additional funding came from Intel Corp. within the activities of the "Research Center for Many-Core HPC" at ZIB, an Intel Parallel Computing Center. The authors acknowledge the North-German Supercomputing Alliance (HLRN) for providing computing time on the Cray XC40.