



Application of HPX to Tiled GEMM and QR: A Benchmark

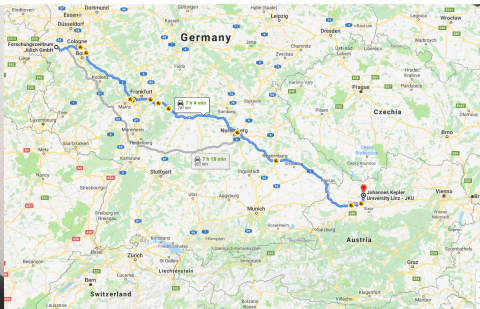
September 25, 2019 | Thomas Miethlinger | Jülich Supercomputing Centre

Part I: Introduction

About me

(Thomas Miethlinger)

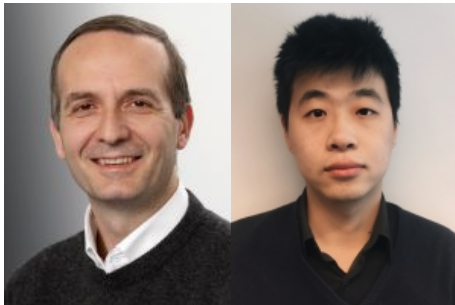
- Study: Master Physics
- Johannes Kepler University of Linz
- Institute for Theoretical Physics
Department: Many Particle Systems
Research:
 - Quantum fluids
 - Complex fluids
 - Non-equilibrium statistical mechanics



About the Supervisors

- Supervisor: Dr. Edoardo Di Napoli
- Co-Supervisor: Dr. Xinzhe Wu
- SimLab Quantum Materials
- Research:
 - Development and maintenance of numerical libraries
 - Design and implementation of high-performance algorithms
 - Development of new mathematical and computational models within a methodological framework

in the scope of computational materials science and quantum materials.



Part II: Introduction to HPX

Current situation in high performance computing (HPC)

Currently, speed-up in computing does not stem from higher CPU frequency, but increased parallelism. However, we already face the following challenges in HPC:

- Ease of programming
- Inability to handle dynamically changing workloads
- Scalability
- Efficient utilization of system resources

⇒ a need for a new execution model: ParalleX, which is implemented by HPX

ParalleX

ParalleX is a new parallel execution model that offers an alternative to the conventional computation models(e.g. message passing):

- Split-phase transaction model
- Message-driven
- Distributed shared memory
- Multi-threaded
- Futures synchronization
- Local Control Objects (LCOs)
- ...

ParalleX focuses on latency hiding instead of latency avoidance.

About HPX

- High Performance ParallelX (HPX) is the first runtime system implementation of the ParallelX execution model.
- Development: STE||AR group
Louisiana State University
LSU Center for Computation and Technology
- Released as open source under the Boost Software License
- Current version: HPX V1.3.0, released on 23.05.2019
- Aims to be a **C++ standards conforming implementation** of the Parallelism and Concurrency proposals for C++ 17/20/23/...
- This means: HPX is a C++ library that supports **dynamic adaptive resource management** and **lightweight task programming and scheduling** within the context of a **global address space**.

On learning HPX

An opinion of a non-CS/HPC student

Learning curve on of HPX is quite steep - in the first days quite some dedication, effort and endurance is needed¹.

- Probably the easiest way in the beginning: watch [this nice playlist](#) in 1.25x speed on the Youtube channel of [cscsch](#) (Swiss National Supercomputing Centre)
- Be aware that the [API reference](#) is not complete
- Be aware that there exist at least 5 different “Hello, World!” examples²:
 - `hpx/examples/hello_world_component/*`: 3 files; 28, 30 & 55 lines
 - `hpx/examples/quickstart/hello_world_1.cpp`; 22 lines
 - `hpx/examples/quickstart/hello_world_2.cpp`; 24 lines
 - `hpx/examples/quickstart/hello_world_distributed.cpp`; 156 lines
 - `tutorials/examples/01_hello_world/hello_world.cpp`; 71 lines

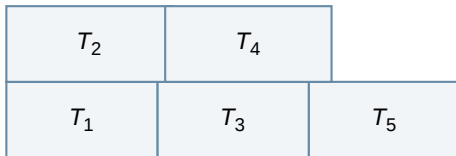
¹Why is the HPX code repo so big and complicated?

²Paths are with respect to <https://github.com/STELLAR-GROUP/>

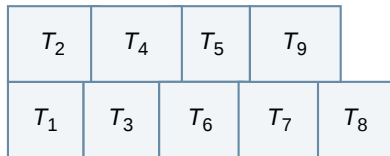
HPX: Tasks and Threads

- HPX: Task-based parallelism
- Split up big problem into smaller tasks
- Tasks are worked off as HPX (lightweight) Threads by the OS Threads
- Task size is crucial: not too small and not too big
- Number of tasks can even be as high as $\mathcal{O}(10^8)$

Tasks too large

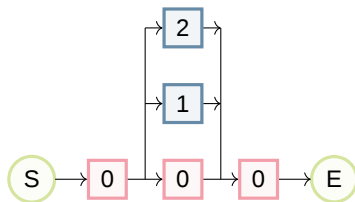
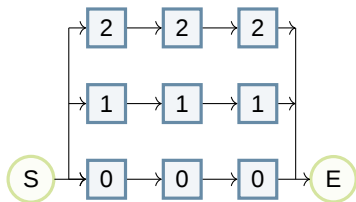


Right task size



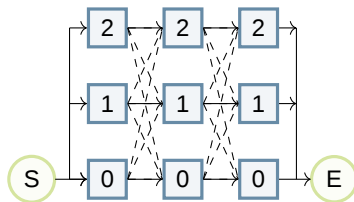
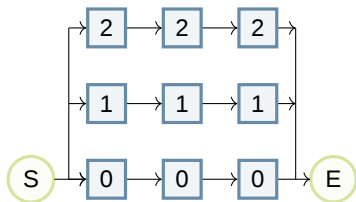
Comparison of HPX and OpenMP

HPX	OpenMP
C++ library Core language: <code>hpx::C++</code> Task-based parallelism AGAS (active global address space)	Compiler extension to C and Fortran <code>#pragma omp</code> directives Parallel regions (fork-join model) Shared memory



Comparison of HPX and MPI

HPX	MPI
C++ library Core language: <code>hpx::C++</code> Task-based parallelism AGAS (active global address space)	Interface specification for C and Fortran Core language: <code>MPI_C</code> , <code>MPI_F08</code> Single program, multiple data (SPMD) Explicit message passing



The HPX API

Selection: Classes

Class	Description
<code>hpx::thread</code>	Low level thread of control
<code>hpx::mutex</code>	Low level synchronization facility
<code>hpx::lcos::local::condition_variable</code>	Signal a condition
<code>hpx::future, hpx::shared_future</code>	Asynchronous result transport (receiving end)
<code>hpx::promise, hpx::lcos::local::promise</code>	Asynchronous result transport (producing end)
<code>hpx::lcos::packaged_task</code>	Asynchronous result transport (producing end)
<code>hpx::function</code>	Type erased function object
<code>hpx::tuple</code>	Tuple
<code>...</code>	

The HPX API

Selection: Functions

Functions	Description
<code>hpx::async</code>	Spawning tasks (returns a future)
<code>hpx::make_ready_future</code>	Spawning tasks (returns a ready future)
<code>hpx::bind</code>	Binding Parameters to callables
<code>hpx::apply</code>	Signal a condition
<code>future::{is_ready, valid, has_exception}</code>	Query state of future
<code>future::get</code>	Return computed result of future
<code>future::then</code>	Continuations of futures
<code>hpx::when_all, hpx::when_any, hpx::when_n</code>	Waiting on one or more futures (non blocking)
<code>hpx::wait_all, hpx::wait_any, hpx::wait_n</code>	Waiting on one or more futures (blocking)
<code>hpx::dataflow</code>	Shortcut to <code>hpx::when_all(...).then(...)</code>
<code>...</code>	

HPX: Example Program

```
double calc_area(hpx::future<double> future_r, hpx::future<double> future_pi)
{
    double r = future_r.get(); // r is returned immediately (make_ready_future)
    double pi = future_pi.get(); // pi is returned once the async computation finishes
    return r * r * pi; // return area = r^2 * pi
}

int hpx_main(variables_map& vm) // In hpx_main the HPX environment is loaded
{
    // boost::program_options::variables_map: retrieve commandline arguments
    hpx::future<double> future_r = hpx::make_ready_future(vm["r"].as<double>());
    hpx::future<double> future_pi = hpx::async([](){ return 4.0 * atan(1.0); });
    hpx::future<double> future_area = hpx::dataflow(&calc_area, future_r, future_pi);
    return hpx::finalize(); // Area can be obtained by: future_area.get()
}

int main(int argc, char * argv[]) // Start program by: ./area --r=...
{
    // boost::program_options::options_description: handle commandline arguments
    options_description.add_options()("r", value<double>()->default_value(1.0), "Radius: r");
    return hpx::init(options_description, argc, argv); // hpx::init calls hpx_main
}
```

Part III: Introduction to Numerical Linear Algebra and Applications

Introduction: Numerical Linear Algebra

Numerical linear algebra is a subfield of numerical analysis and linear algebra, and it plays an integral role in computational problem solving. There exist many several algorithms for common problems, a few well-known are:

- Solving systems of linear equations
- Eigenvalue problem
- Matrix inversion problem
- Least-squares problem

which may be using one of the following matrix operations/decompositions:

- Matrix multiplications
- LU decomposition
- QR decomposition
- Spectral decomposition
- Singular value decomposition

Part IV: GEMM

GEMM

Applications of Numerical Linear Algebra

GEMM - GEneral Matrix Multiply

- Basic binary operation in Linear Algebra, which has numerous applications in mathematics, science and engineering.
- More fundamental applications of matrix multiplications include
 - Systems of Linear Algebraic Equations (SLAE) can be expressed as a single matrix equation, e.g. $Ax = y$.
 - Linear map between two vector spaces U and V over the same field F .
- Motivation: A large amount (>70%) of runtime in ChASE ((E.D. Napoli, 2019)) routine is used for GEMM.
- Let the field F be \mathbb{R} or \mathbb{C} , $A = (a_{ij}) \in F^{m \times n}$, $B = (b_{jk}) \in F^{n \times p}$. Then,

$$C = (c_{ik}) = AB \in F^{m \times p}, \quad (1)$$

$$c_{ik} = \sum_{j=1}^n a_{ij} b_{jk} \quad (2)$$

GEMM of Blocked Matrices

Applications of Numerical Linear Algebra

⇒ most simple implementation consists of 3 nested for-loops:

for $0 \leq i < m$, $0 \leq j < n$, $0 \leq k < p$, do: $C[i][k] += A[i][j] * B[j][k]$

Better approach: Discretize matrices into blocks, perform GEMM **block-wise**

Let the field F again be \mathbb{R} or \mathbb{C} , $A = (A_{ij}) \in F^{M \times N \times m \times n}$, $B = (B_{jk}) \in F^{N \times P \times n \times p}$.

Then:

$$C = (C_{ik}) = AB \in F^{M \times P \times m \times p}, \quad (3)$$

$$C_{ik} = (c_{ik,i'k'}) = \sum_{j=1}^n A_{ij} B_{jk}, \quad (4)$$

$$c_{ik,i'k'} = \sum_{j=1}^N \sum_{j'=1}^n a_{ij,i'j'} b_{jk,j'k'} \quad (5)$$

A Small Example

Let $M = N = P = m = n = p = 2$:

$$\begin{array}{ccc} \boxed{A} & \cdot & \boxed{B} = \boxed{C} \\ \begin{array}{|c|c|} \hline A_{00} & A_{10} \\ \hline A_{01} & A_{11} \\ \hline \end{array} & \cdot & \begin{array}{|c|c|} \hline B_{00} & B_{10} \\ \hline B_{01} & B_{11} \\ \hline \end{array} = \begin{array}{|c|c|} \hline C_{00} & C_{10} \\ \hline C_{01} & C_{11} \\ \hline \end{array} \end{array}$$

A Small Example

Let $m = n = p = M = N = P = 2$:

$$\begin{array}{ccc} \boxed{A_{ij}} & \cdot & \boxed{B_{jk}} = \boxed{A_{ij}B_{jk}} \\ \begin{array}{|c|c|} \hline a_{ij,00} & a_{ij,10} \\ \hline a_{ij,01} & a_{ij,11} \\ \hline \end{array} & \cdot & \begin{array}{|c|c|} \hline b_{jk,00} & b_{jk,10} \\ \hline b_{jk,01} & b_{jk,11} \\ \hline \end{array} = \begin{array}{|c|c|} \hline \dots & \dots \\ \hline \dots & \dots \\ \hline \end{array} \end{array}$$

Part V: QR

QR decomposition

Applications of Numerical Linear Algebra

QR decomposition

- Matrix decomposition of square or rectangular matrices (we only consider square matrices).
- Let the field F be \mathbb{R} or \mathbb{C} , $A = (a_{ij}) \in F^{m \times m}$. Then,

$$A = QR, \tag{6}$$

where Q is a orthogonal($F = \mathbb{R}$) / unitary($F = \mathbb{C}$) matrix, and R is an upper triangular matrix.

- Motivation: A large amount (>20%) of runtime in ChASE (([ED Napoli, 2019](#))) routine is used for QR.
- Computing the QR decomposition:
 - Gram-Schmidt process
 - **Householder reflection**
 - Givens rotations

Applications of QR decomposition

Examples

- Computing Eigenvalues (QR algorithm)
- Computing orthogonal base
- Solving least-squares problem
- Solution to linear inverse problems

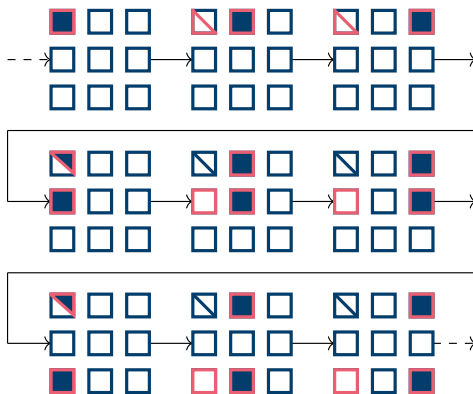
A selection of papers within the scope of my research interest which use QR decomposition:

- An evaluation of noise reduction algorithms for particle-based fluid simulations in multi-scale applications ([M.J. Zimon et al., 2016](#))
- Dynamic mode decomposition of numerical and experimental data ([P.J. Schmid, 2010](#))
- Krylov Methods for the Incompressible Navier-Stokes Equations ([W.S. Edwards, 1994](#))
- Computing Lyapunov exponents of continuous dynamical systems: method of Lyapunov vectors ([J. Lu, 2005](#))

QR decomposition

Algorithm: Householder Reflection

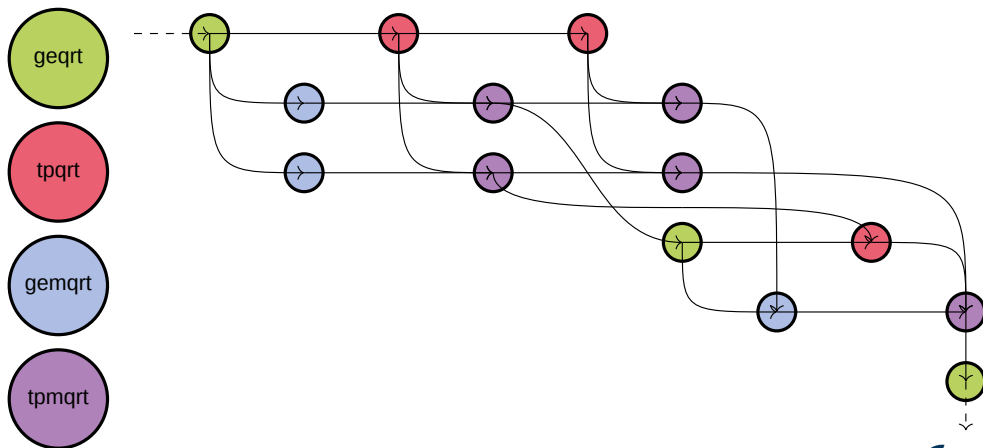
Example: $3 \times 3 \times 3 \times 3$ block matrix.



QR decomposition

Algorithm: Householder Reflection

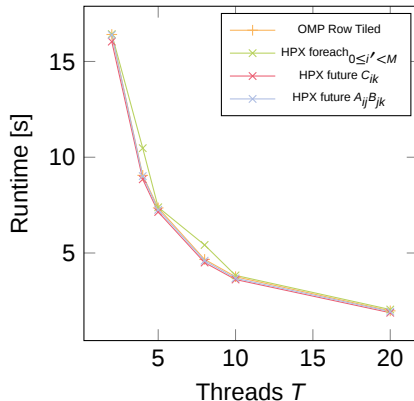
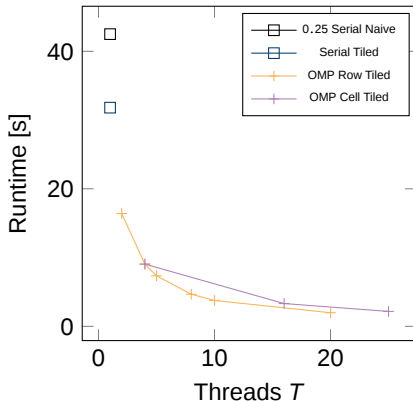
Example: $3 \times 3 \times 3 \times 3$ block matrix.



Part VI: Benchmark: Results for GEMM

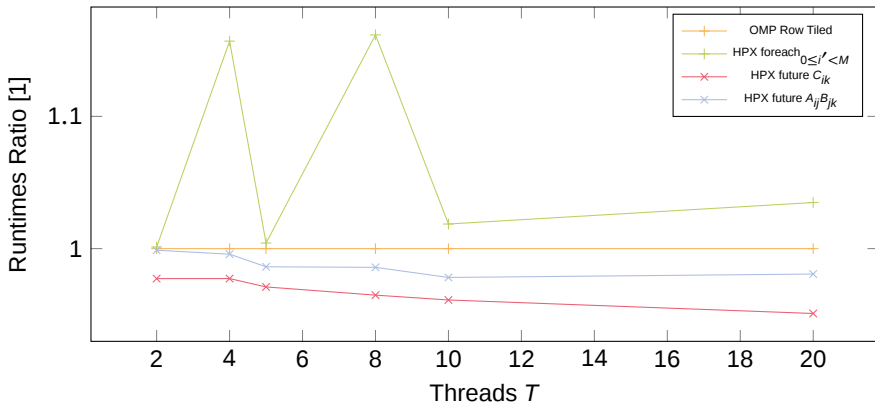
GEMM Shared Memory

Let $m = n = p = 4000$, $M = N = P = 40$, vary number of threads:



GEMM Shared Memory

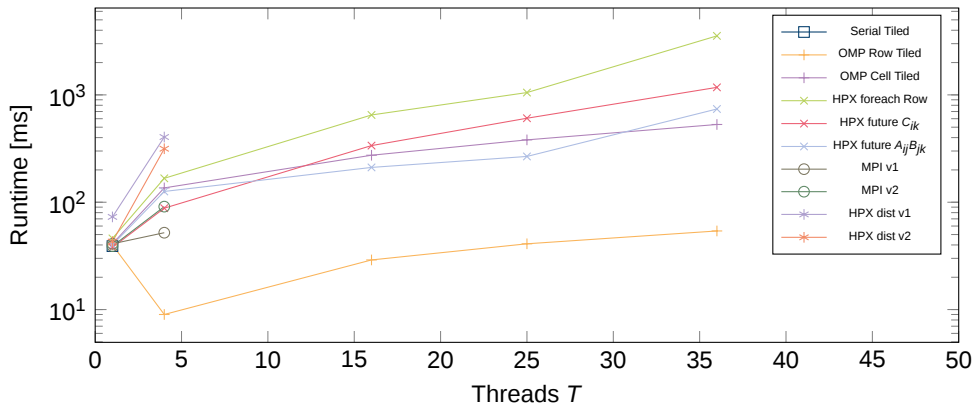
Let $m = n = p = 4000$, $M = N = P = 40$, vary number of threads:



⇒ HPX can be faster than OpenMP, even for embarrassingly parallel problems, in particular `hpx::futures`.

GEMM

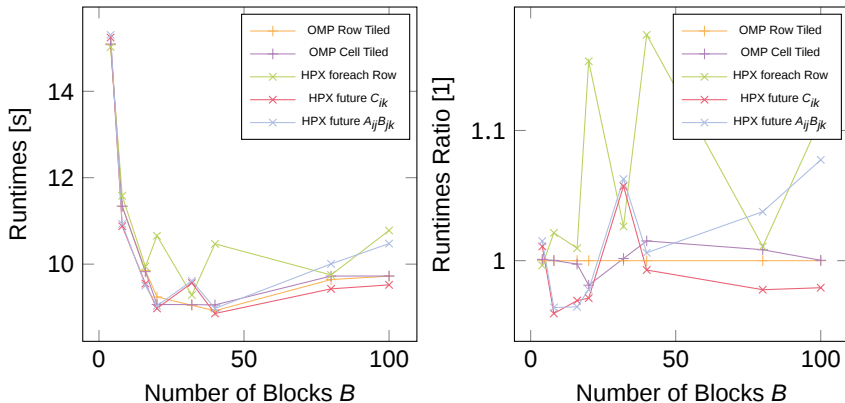
Vary number of threads T , and let $m = n = p = 400\sqrt{T}$, $M = N = P = \sqrt{T}$:



- Task-size crucial for HPX. Here the block size was too big.
- HPX distributed is quite slower than MPI. The implementations are equivalent/analogous.

GEMM Shared Memory

Let $m = n = p = 4000$, $T = 4$, vary number of blocks $B := M = N = P$:

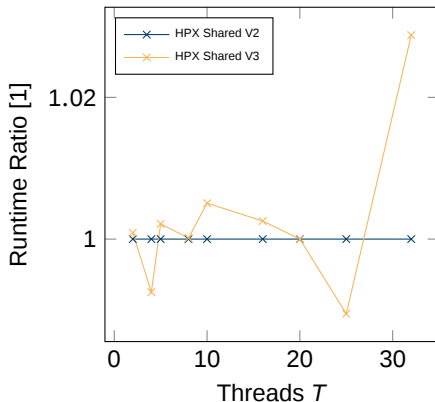
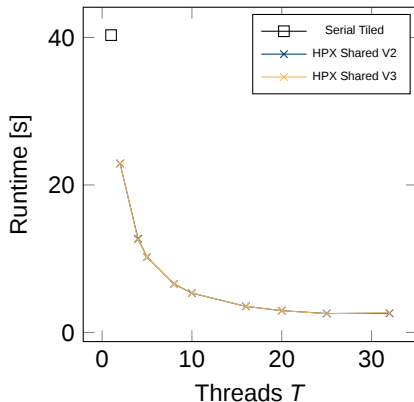


⇒ Again, HPX is around the same speed as OpenMP.

Part VII: Benchmark: Results for QR

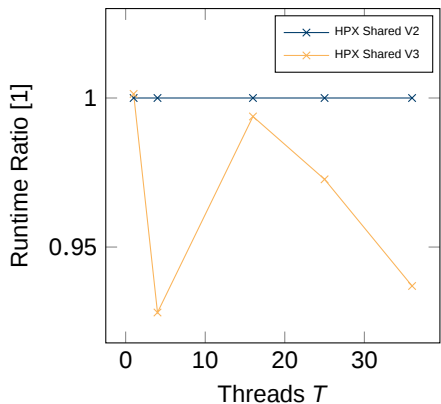
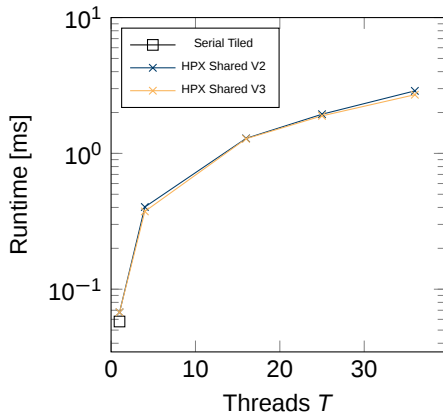
QR Shared Memory

Let $m = 4000$, $M = 40$, vary number of threads:



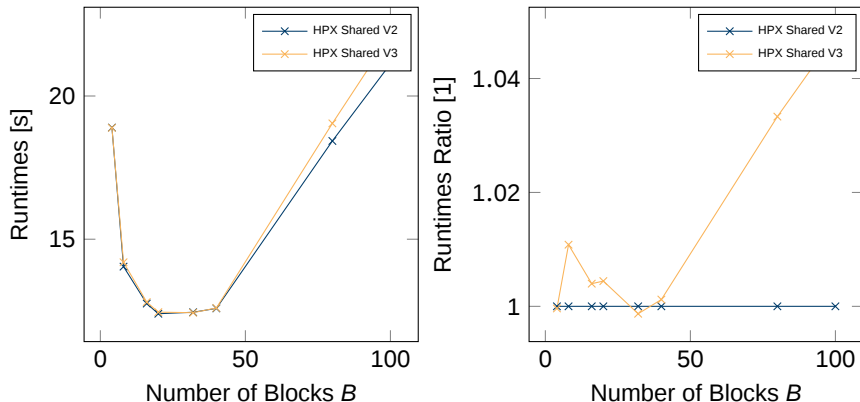
QR Shared Memory

Vary number of threads T , and let $m = n = p = 400\sqrt{T}$, $M = N = P = \sqrt{T}$:



GEMM Shared Memory

Let $m = n = p = 4000$, $T = 4$, vary number of blocks $B := M = N = P$:



Part VIII: Conclusion and Resume

Conclusion

On HPX

- HPX has the potential to speed-up and simplify parallelization for certain types of problems
- On par with OpenMP
- Comparison with MPI unfortunately not possible at this moment
- Learning HPX takes some time, in particular HPX for distributed programs
- Debugging, profiling, runtime errors, documentation, ... could be improved
- Execution policies: might give additional speed-up
- Altogether: Very strong library and concept with some negative points

Resume

Personal thoughts

- Interesting project, work and topic. I learned a lot.
- Collaboration with Dr. Wu worked very well. Thanks!
- On HPX
 - * Some fun
 - * Takes a medium amount of time
 - + Full C++ library
 - Bugs can be nasty
- On MPI
 - + Lots of fun
 - Takes a lot of time
 - No native C++
 - * Usually works, and if not, it is manageable to figure out why
- On OpenMP
 - No fun
 - + Doesn't take a lot of time
 - + Simply works :)



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