

# **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





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### **About the Supervisors**

Supervisor: Dr. Edoardo Di Napoli

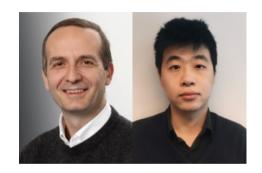
Co-Supervisor: Dr. Xinzhe Wu

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.





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# **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):

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- 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 ParalleX (HPX) is the first runtime system implementation of the ParalleX 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 needed<sup>1</sup>.

- 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!" examples<sup>2</sup>:
  - 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



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<sup>&</sup>lt;sup>1</sup>Why is the HPX code repo so big and complicated?

<sup>&</sup>lt;sup>2</sup>Paths 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  $\mathcal{O}(10^8)$

T <sub>2</sub>	$T_4$	
<i>T</i> <sub>1</sub>	T <sub>3</sub>	T <sub>5</sub>

Tasks too large

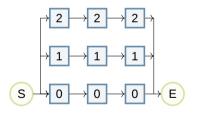
#### Right task size

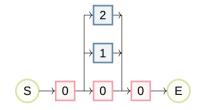
<i>T</i> <sub>2</sub>	T <sub>4</sub>	T <sub>5</sub>	$T_9$	
<i>T</i> <sub>1</sub>	<i>T</i> <sub>3</sub>	$T_6$	<i>T</i> <sub>7</sub>	T <sub>8</sub>



# **Comparison of HPX and OpenMP**

HPX	OpenMP
C++ library	Compiler extension to C and Fortran
Core language: hpx::C++	#pragma omp directives
Task-based parallelism	Parallel regions (fork-join model)

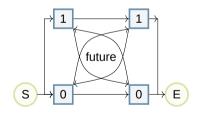


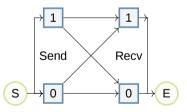




# **Comparison of HPX and MPI**

HPX	MPI
C++ library	Interface specification for C and Fortran
Core language: hpx::C++	Core language: MPI_C, MPI_F08
Task-based parallelism	Single program, multiple data (SPMD)
Message driven	Message passing







#### The HPX API

Selection: Classes

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



#### The HPX API

**Selection: Functions** 

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



#### **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.qet(); // 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, GEMM and QR



### **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



#### **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,

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

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



#### **GEMM of Blocked Matrices**

#### **Applications of Numerical Linear Algebra**

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

for 
$$0 \le i \le m$$
,  $0 \le j \le n$ ,  $0 \le k \le p$ , 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:

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

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

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



# **A Small Example**

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

Α

=

C

 $A_{00}$   $A_{10}$   $A_{01}$   $A_{11}$ 

 $B_{00}$   $B_{10}$   $B_{01}$   $B_{11}$ 

=

 $C_{00}$   $C_{10}$   $C_{01}$ 

# **A Small Example**

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



 $b_{jk,11}$ 

$$A_{ij}B_{jk}$$

$$a_{ij,00}$$
  $a_{ij,10}$   $a_{ij,11}$ 

$$b_{jk,00}$$
  $b_{jk,10}$   $b_{jk,11}$ 

### **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,

$$A = QR, (6)$$

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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 ((E.D. 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

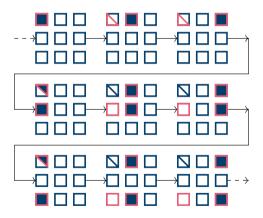
A selection of papers within the scope of my research interest which use QR decomposition:

- 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)



### **Block QR decomposition**

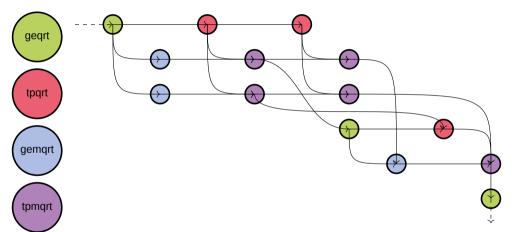
Example: 3 × 3 block matrix





# **Block QR decomposition**

Example: 3 × 3 block matrix

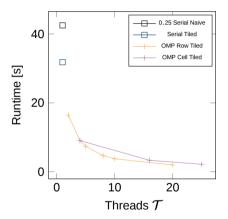


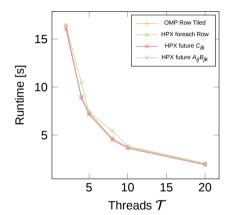


# Part IV: Benchmark: Results for GEMM



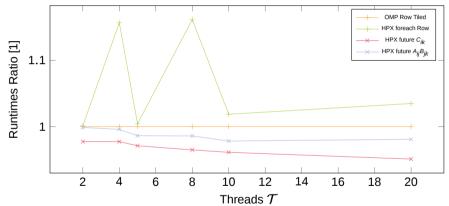
Let m = n = p = 4000, M = N = P = 40, vary number of threads T:







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

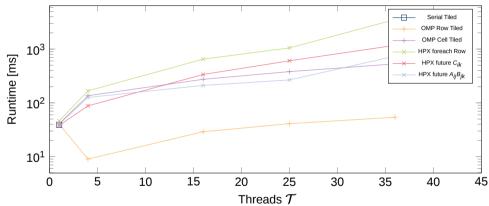


 $\implies$  HPX can be faster than OpenMP, even for embarrassingly parallel problems, in particular

hpx::futures.

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

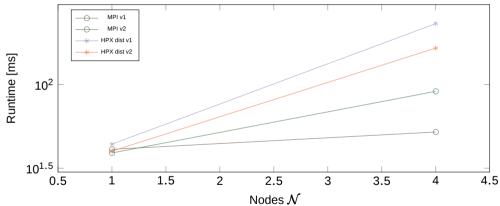


→ Task-size crucial for HPX. Here the block size was too big.



### **GEMM Distributed Memory**

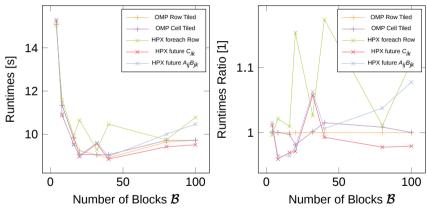
Vary number of Nodes  $\mathcal{N}$ , and let  $m=n=p=400\sqrt{\mathcal{N}}$ ,  $M=N=P=\sqrt{\mathcal{N}}$ :



HPX distributed is slower than MPI, their implementations are presumably analogous.



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



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

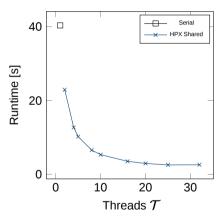


# Part V: Benchmark: Results for Tiled QR



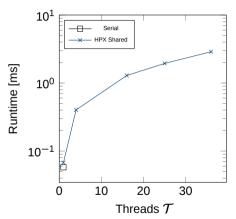
### **QR Shared Memory**

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



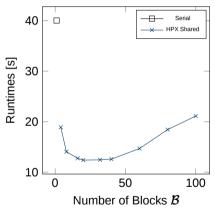
# **QR Shared Memory**

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



### **QR Shared Memory**

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



⇒ Discretizing problem into blocks has a high impact on runtime!



# **Part VI: 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 (supplemented for report)
- 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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