

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 GSP

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 sitution 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 focusses 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.



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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



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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 $\mathcal{O}(10^8)$

T ₂	T_4	
<i>T</i> ₁	T ₃	T ₅

Tasks too large

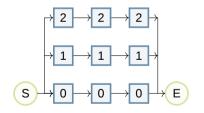
Right task size

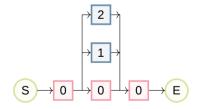
T ₂	T ₄	<i>T</i> ₅	<i>T</i> ₉	
T_1	<i>T</i> ₃	T_6	<i>T</i> ₇	T ₈



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)
AGAS (active global address space)	shared memory

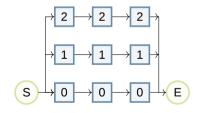


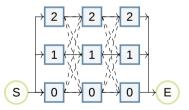




Comparison of HPX and MPI

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)
AGAS (active global address space)	Explicit 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:
int hpx_main(variables_map& vm) // In hpx_main the HPX environment is loaded
   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=...
   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.
 - 2 Linear map between two vector spaces U and V over the same field F.
- Motivation: A large amount (>70%) of runtime in ChASE ((ED 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:

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

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

A Small Example

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

 A_{ij}

 B_{jk}

=

 $A_{ij}B_{jk}$

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

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

=



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,

$$A = QR, (6)$$

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

- Computing the QR decomposition:
 - Gram-Schmidt orthogonalisation 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 in my research ares 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

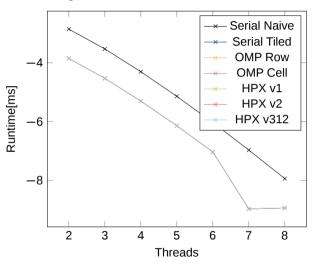
Algorithm



Part VI: Benchmark: Results

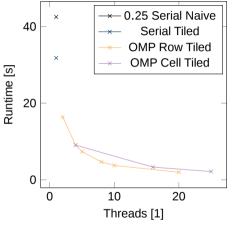


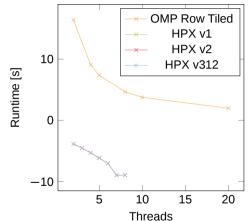
GEMM Shared Memory





GEMM Shared Memory







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