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

$\Longrightarrow$ 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**.

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[1].

- 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[2]:
  - 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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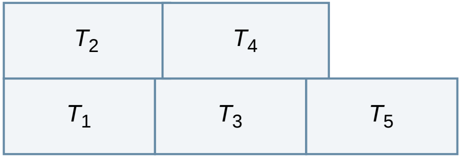
[1] Why is the HPX code repo so big and complicated?

[2] Paths are with respect to `https://github.com/STEllAR-GROUP/`

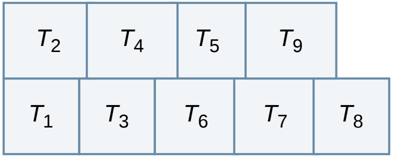
HPX: Tasks and Threads

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

Tasks too large

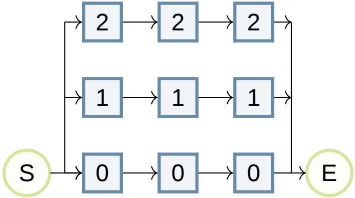


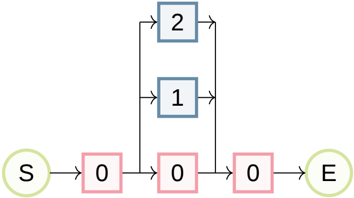
Right task size



Comparison of HPX and OpenMP

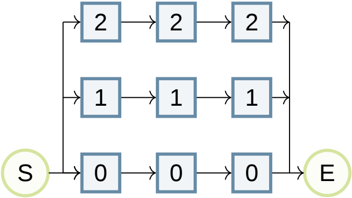
HPX	OpenMP
C++ library Core language: `hpx::C++` Task-based parallelism AGAS (active global address space)	Compiler extension to C and Fortran `#pragma omp` directives Parallel regions (fork-join model) shared memory

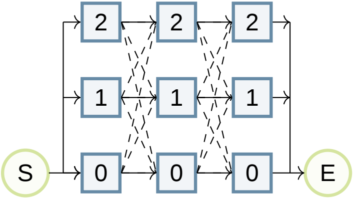




Comparison of HPX and MPI

HPX	MPI
C++ library Core language: `hpx::C++` Task-based parallelism AGAS (active global address space)	Interface specification for C and Fortran Core language: MPI_C, MPI_F08 Single program, multiple data (SPMD) 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
`future::{is_ready, valid, has_exception}`	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.get(); // 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
  1. 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 $\mathbb{C}$, $A = \left(a_{ij}\right) \in F^{m\times n}$, $B = \left(b_{jk}\right) \in F^{n\times p}$. Then,

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

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

GEMM of Blocked Matrices

Applications of Numerical Linear Algebra

$\Longrightarrow$ most simple implementation consists of 3 nested for-loops:

```
for 0 <= i < m, 0 <= j < n, 0 <= 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 $\mathbb{C}$, $A = \left(A_{ij}\right) \in F^{M \times N \times m \times n}$, $B = \left(B_{jk}\right) \in F^{N \times P \times n \times p}$.

Then:

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

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

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

A Small Example

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

$$A \cdot B = C$$

$$\begin{bmatrix} A_{00} & A_{10} \\ A_{01} & A_{11} \end{bmatrix} \cdot \begin{bmatrix} B_{00} & B_{10} \\ B_{01} & B_{11} \end{bmatrix} = \begin{bmatrix} C_{00} & C_{10} \\ C_{01} & C_{11} \end{bmatrix}$$

A Small Example

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

$$\boxed{A_{ij}} \cdot \boxed{B_{jk}} = \boxed{A_{ij}B_{jk}}$$

$$\begin{array}{|c|c|}\hline a_{ij,00} & a_{ij,10} \\ \hline a_{ij,01} & a_{ij,11} \\ \hline \end{array} \cdot \begin{array}{|c|c|}\hline b_{jk,00} & b_{jk,10} \\ \hline b_{jk,01} & b_{jk,11} \\ \hline \end{array} = \begin{array}{|c|c|}\hline \cdots & \cdots \\ \hline \cdots & \cdots \\ \hline \end{array}$$

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 $\mathbb{C}$, $A = \left(a_{ij}\right) \in F^{m \times m}$. 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.
- 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:

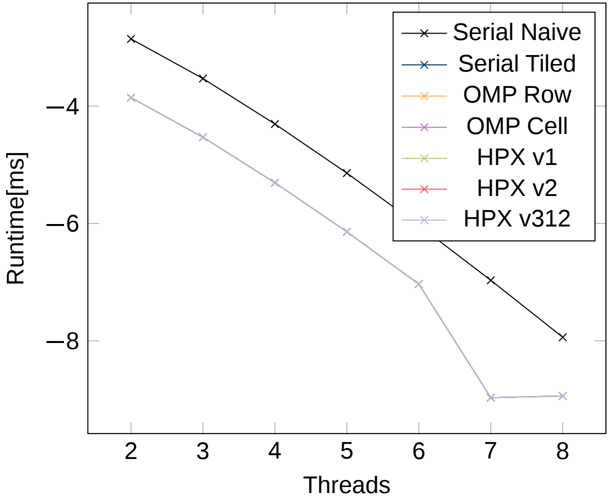
- An evaluation of noise reduction algorithms for particle-based fluid simulations in multi-scale applications (M.J. Zimon et al., 2016)
- Dynamic mode decomposition of numerical and experimental data (P.J. Schmid, 2010)
- Krylov Methods for the Incompressible Navier-Stokes Equations (W.S. Edwards, 1994)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

QR decomposition

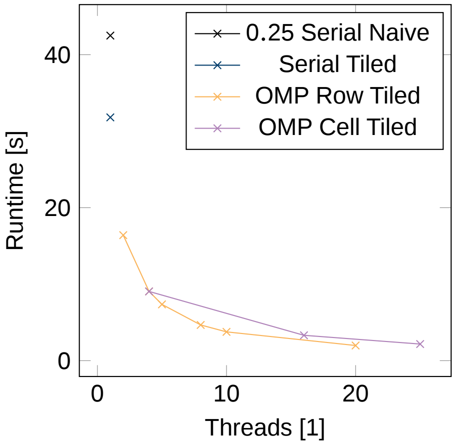
Algorithm

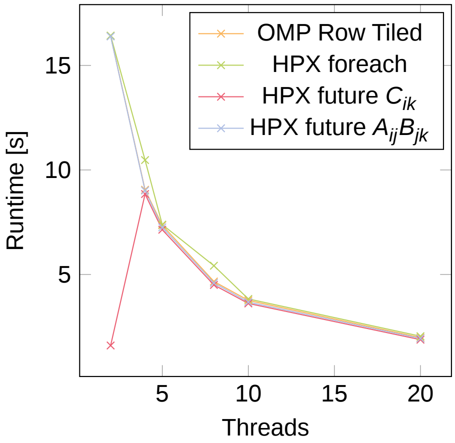
Part VI: Benchmark: Results

GEMM Shared Memory



GEMM Shared Memory





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