Alternative Programming Models
Distributed tasking with PaRSEC

George Bosilca and many others

BSC, Nov, 2018
Exponential growth in HPC

• Appetite for compute will continue to grow exponentially
• Fueled by the need to solve many fundamental problems and deal with a growing amount of data
  • Energy, weather forecast, health, understanding the universe but also connected devices, deep learning
• The path forward seems to be a mix of many-core general purpose supported by special purpose units (not necessarily computation only)
• New challenges arise: power, space, cost, reliability, memory, ...
  • But also software
  • Hardware solutions that require major changes in software ecosystem are less likely to gain widespread acceptance [quickly]
A [very brief] history of computing paradigms

BSP & early message passing

MPI + X

MPI + X + Y + Z + ...

Concurrency*

Heterogeneity

Resiliency
A [very brief] history of computing paradigms

- BSP & early message passing
- MPI + X
- MPI + X + Y + Z + ...

Concurrency*
Heterogeneity
Resiliency

In the diagram, the x-axis represents the number of pairs of processes or threads, and the y-axis represents the injection rate. The legend indicates two types of communication: Process to Process and Thread to Thread. The graph shows a comparison of injection rates with different bandwidth scenarios, with a peak of 40X gain in process communication.
A [very brief] history of computing paradigms

- Heterogeneity
- Concurrency
- Resiliency

BSP & early message passing

MPI + X

MPI + X + Y + Z + ...

Higher better

process

40X

4X

3X

thread Optimized 1 sided MPI

thread Optimized 2 sided MPI

thread
A [very brief] history of computing paradigms

- Over-subscription:
  - User level threads (Qthreads, MassiveThreads, Nanos++, Argobots)

- Task-ification:
  - Shared memory: OpenMP, Tascel, Quark, TBB*, PPL, Kokkos**, SuperGluer...
  - Distributed Memory: StarPU, StarSS*, DARMA**, Legion, CnC, HPX, Dagger, X10, DuctTeip, Hihat**, ...
    * explicit communications
    ** nascent effort

- Difficult to express the potential inter-algorithmic parallelism
  - Why are we still struggling with control flow?
  - Software became an amalgam of algorithm, data distribution and architecture characteristics

- Increasing gaps between the capabilities of today’s programming environments, the requirements of emerging applications, and the challenges of future parallel architectures

- What about developers productivity?
Task-based programming support

<table>
<thead>
<tr>
<th>Year</th>
<th>System</th>
<th>Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>1992</td>
<td>MPI</td>
<td>More of a communication library than a runtime, Explicit communication</td>
</tr>
<tr>
<td>1993</td>
<td>Charm++</td>
<td>Supports distributed memory, Low level – not based on dataflow (explicit)</td>
</tr>
<tr>
<td>2010</td>
<td>DAGuE/PaRSEC</td>
<td>Supports distributed memory, Data-flow based, Implicit communication</td>
</tr>
<tr>
<td>2012</td>
<td>Legion</td>
<td>Nascent support for distributed memory, Data-flow based</td>
</tr>
<tr>
<td>2013</td>
<td>Legion</td>
<td>Supports distributed memory, Focus on compiler to allow programmer express applications more easily</td>
</tr>
<tr>
<td>2014</td>
<td>OpenMP</td>
<td>Introduces dependency tracking for tasks in Standard 4</td>
</tr>
<tr>
<td>2015</td>
<td>StarPU</td>
<td>Supports distributed memory, Performance most close to DTD</td>
</tr>
<tr>
<td>2016</td>
<td>StarPU</td>
<td>Supports shared memory, Communication possible through tasks(explicit)</td>
</tr>
<tr>
<td>2017</td>
<td>PaRSEC insert_task(DTD)</td>
<td></td>
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</tbody>
</table>

This diagram illustrates the evolution of task-based programming support, highlighting the introduction and features of various systems throughout the years.
**PaRSEC**: a generic runtime system for asynchronous, architecture aware scheduling of fine-grained tasks on distributed many-core heterogeneous architectures

### Concepts
- Clear separation of concerns: **compiler optimize** each task class, **developer describe** dependencies between tasks, the **runtime orchestrate** the dynamic execution
- Interface with the application developers through specialized domain specific languages (PTG/JDF/TTG, Python, insert_task, fork/join, …)
- Separate algorithms from data distribution
- Make control flow executions a relic

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### Runtime
- Portability layer for heterogeneous architectures
- Scheduling policies adapt every execution to the hardware & ongoing system status
- Data movements between producers and consumers are inferred from dependencies. Communications/computations overlap naturally unfold
- Coherency protocols minimize data movements
- Memory hierarchies (including NVRAM and disk) integral part of the scheduling decisions
PaRSEC = a data centric programming environment based on asynchronous tasks executing on a heterogeneous distributed environment

- An execution unit taking a set of input data and generating, upon completion, a different set of output data
- Data have a coherent distributed scope managed by the runtime (similar to promises)
- Low-level API allowing the design of Domain Specific Languages (JDF, DTD, TTG)
- Supports distributed heterogeneous environments
  - Communications are implicit (the runtime moves data)
  - Resources (threads, accelerators) are dynamic encapsulated in distributed domains (similar to executors)
  - Built-in resilience, performance instrumentation and analysis (R, python)
PaRSEC Architecture

Software design based on Modular Component Architecture (MCA) of Open MPI.

- Well defined components API
- Runtime selection of components
- Providing a new capability by implementing a new component has no impact on the rest of the software stack.
  - Can be provided as dynamic libraries by vendors
The PaRSEC data

- A data is a manipulation token, the basic logical element (view) used in the description of the dataflow
  - Locations: have multiple coherent copies (remote node, device, checkpoint)
  - Shape: can have different memory layout
  - Visibility: only accessible via the most current version of the data
  - State: can be migrated / logged
- **Data collections** are ensemble of data distributed among the nodes
  - Can be regular (multi-dimensional matrices)
  - Or irregular (sparse data, graphs)
  - Can be regularly distributed (cyclic-k) or user-defined
- **Data View** a subset of the data collection used in a particular algorithm (aka. submatrix, row, column,...)

- A data-copy is the practical unit of data
  - Has a memory layout (think MPI datatype)
  - Has a property of locality (device, NUMA domain, node)
  - Has a version associated with
  - Multiple instances can coexist
DSL: The PaRSEC application

Define a distributed collection of data (here 1 dimension array of integers)

Start PaRSEC (resource allocation)

Create a tasks placeholder and associate it with the PaRSEC context

Add tasks. A configurable window will limit the number of pending tasks

Wait 'till completion

```c
parsec_vector_t dDATA;
parsec_vector_init( &dDATA, matrix_Integer, matrix_Tile,
    nodes, rank,
    1, /* tile_size*/
    N, /* Global vector size*/
    0, /* starting point */
    1 ); /* block size */
```

```c
parsec_context_t* parsec;
parsec = parsec_context_init(NULL, NULL); /* start the PaRSEC engine */
```

```c
parsec_taskpool_t* ts = parsec_taskpool_new();
parsec_context_add_taskpool (parsec, ts);
parsec_context_start (parsec);
```

```c
parsec_context_wait (parsec);
```
How to describe a graph of tasks?

- Uncountable ways
  - Generic: Dagguer (Charm++), Legion, ParalleX, Parameterized Task Graph (PaRSEC), Dynamic Task Discovery (StarPU, StarSS), Yvette (XML), Fork/Join (spawn), CnC, Uintah, DARMA, Kokkos, RAJA, OMPSS
  - Application specific: MADNESS, ...

- PaRSEC runtime
  - The runtime is agnostic to the domain specific language (DSL)
  - Different DSL interoperate through the data collections
  - The DSL share
    - Distributed schedulers
    - Communication engine
    - Hardware resources
    - Data management (coherence, versioning, ...)
  - They don’t share
    - The task structure
  - The internal dataflow depiction
**DSL: The insert_task interface**

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parsec_context_t* parsec;
parsec = parsec_context_init(NULL, NULL);  /* start the PaRSEC engine */

parsec_taskpool_t* ts = parsec_taskpool_new();
parsec_context_add_taskpool (parsec, ts);

parsec_context_start(parsec);

for( n = 0; n < N; n++ ) {
    parsec_insert_task( ts,
        call_to_kernel_type_write, "Create Data",
        PASSED_BY_REF, DATA_AT(dDATA, n), OUT | REGION_FULL,
        0 /* DONE */);
    for( k = 0; k < K; k++ ) {
        parsec_insert_task( ts,
            call_to_kernel_type_read, "Read_Data",
            PASSED_BY_REF, DATA_AT(dDATA, n), INPUT | REGION_FULL,
            0 /* DONE */);
    }
}

parsec_context_wait(parsec);
```
for( k = 0; k < SIZE; k++ ) {
    insert_task( "GEQRT",
        DATA_OF(A, k, k),
        DATA_OF(T, k, k),
        INOUT|AFFINITY,
        OUTPUT|TILE_RECT)

    for( n = k+1; n < SIZE; n++ )
        insert_task( "UNMQR",
            DATA_OF(A, k, k),
            DATA_OF(A, k, n),
            DATA_OF(T, k, k),
            DATA_OF(T, k, n),
            INPUT|TILE_L,
            INPUT|TILE_RECT,
            INPUT|AFFINITY,
            INOUT|AFFINITY)

    for( m = k+1; m < SIZE; m++ ) {
        insert_task( "TSQRT",
            DATA_OF(A, k, k),
            DATA_OF(A, m, k),
            DATA_OF(A, m, n),
            DATA_OF(T, m, k),
            DATA_OF(T, m, k),
            INOUT|TILE_U,
            INOUT|AFFINITY,
            OUTPUT|TILE_RECT)

        for( n = k+1; n < SIZE; n++ )
            insert_task( "TSMQR",
                DATA_OF(A, k, n),
                DATA_OF(A, m, n),
                DATA_OF(A, m, k),
                DATA_OF(T, m, k),
                DATA_OF(T, m, k),
                INOUT,
                INOUT|AFFINITY,
                INPUT,
                INPUT|TILE RECT)
for( k = 0; k < SIZE; k++ ) {
  insert_task( "GEQRT", DATA_OF(A, k, k), INOUT|AFFINITY, DATA_OF(T, k, k), OUTPUT|TILE_RECT)
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  for( m = k+1; m < SIZE; m++ )
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  for( n = k+1; n < SIZE; n++ )
    insert_task( "TSMQR", DATA_OF(A, k, n), INOUT, DATA_OF(A, m, n), INOUT|AFFINITY, DATA_OF(A, m, k), INPUT, DATA_OF(T, m, k), INPUT|TILE_RECT)
}
}
Overhead of insert_task

\[ T_{DTD} = \frac{N \times C_T}{P \times n} + N \times C_D + \frac{N \times C_R}{P} \]

- **DTD overhead**

- **Benefits**: critical path is defined by the sequential ordering
- **Drawbacks**: impossible to build collective patterns, selecting the window size is difficult, all data movement must be known globally (and their order is critically important)

- **There are three types of scenario**
  - Insert All: Each rank inserts all tasks, and executes only locals
  - Select Insert: Each rank inserts only local tasks, but iterates over all tasks.
  - Insert Local: Each rank only inserts local tasks.

- **Fixed task duration**
- **Weak scaling**: Fixed number of tasks per process

- **Stampede2**: 3 cores/process, 128 Nodes

- **6144 cores**
What’s missing from insert_task?

• Need to balance between task graph knowledge and memory overhead
  • The task graph creation must happen in a single thread

• To trim or not to trim? Who is tracking the data in order to orchestrate global data coherence?

• Difficult to type the input and output data, especially if one expects the dependencies to only apply on partial data

• Difficult to reliably expose collective patterns without complete knowledge of the task graph as different processes might have discovered different sections of the task graph
PaRSEC DSL comparaison

Problem Scaling: DPOTRF, Tile: 320, Nacl 64 nodes, 8x8

GFlops

0 1000 2000 3000 4000 5000 6000

Size

20000 40000 60000 80000 100000 120000

dpotrf_dplasma_dtd
scalapack_impi

VS.
VS.

Motivation
Related Works
The DAGuE framework
Performance Evaluation
Conclusion

Micro Benchmarking
Application: Cholesky Decomposition

Illustration of the Talk:
Cholesky Factorization
20 x 20 tiles matrix
George Bosilca
DAGuE vs.
vs.
SLATE (over PaRSEC) approach

- Back to the future: return to the ScaLAPACK approach, the problem hierarchically divided (panel + update) with flexible lookahead
- Remove most data dependencies (except data movement and versioning)
  - The design is flexible enough to allow good performance on runtimes with high scheduling costs (such as OpenMP or StarPU)
- Variable granularity with several benefits: task duration, task location, well exposed “batched” operation
  - Potential benefit for accelerators
- Present a different view to data movement
  SLATE.send(data, [data range]+)
  - Explicit life-expectancy for remote data
  - Expose collective communications
- Everything is done in templated C++11, but the resulting programming model (DSL) is generic
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George Bosilca
DAGuE
vs.

Preliminary results
The Parameterized Task Graph (PTG/JDF)

\[
\text{GEQRT}(k)
\]

\[
k = 0..(\text{MT} < \text{NT}) ? \text{MT}-1 : \text{NT}-1
\]

\[
: A(k, k)
\]

\[
\text{RW } A <- (k == 0) ? A(k, k) : A1 \text{TSMQR}(k-1, k, k)
\]

\[
-> (k < \text{NT}-1) ? A \text{UNMQR}(k, k+1 .. \text{NT}-1) \quad \text{[type = LOWER]}
\]

\[
-> (k < \text{MT}-1) ? A1 \text{TSQRT}(k, k+1) \quad \text{[type = UPPER]}
\]

\[
-> (k == \text{MT}-1) ? A(k, k) \quad \text{[type = UPPER]}
\]

\[
\text{WRITE } T <- T(k, k)
\]

\[
-> T(k, k)
\]

\[
-> (k < \text{NT}-1) ? T \text{UNMQR}(k, k+1 .. \text{NT}-1)
\]

\[
\text{BODY [type = CPU] /* default */}
\]

\[
zgeqrt( A, T );
\]

\[
\text{END}
\]

\[
\text{BODY [type = CUDA]}
\]

\[
cuda\_zgeqrt( A, T );
\]

\[
\text{END}
\]

- A dataflow parameterized and concise language
- Accept non-dense iterators
- Allow inlined C/C++ code to augment the language [any expression]
- Termination mechanism part of the runtime (i.e. needs to know the number of tasks per node)
- The dependencies had to be globally (and statically) defined prior to the execution
- Dynamic DAGs non-natural
- No data dependent DAGs

Control flow is eliminated, therefore maximum parallelism is possible.
PaRSEC DSL comparaison

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20 x 20 tiles matrix

George Bosilca
DAGuE

Preliminary results

Problem Scaling: DPOTRF, Tile: 320, Nacl 64 nodes, 8x8

Gflops vs. Size

- dpotrf_dplasma_dtd
- dpotrf_slate_master
- dpotrf_dplasma_ptg
- scalapack_impi
- dpotrf_slate_dtd

vs. vs.
Experiments on Arc machines,
  • E5-2650 v3 @ 2.30GHz
  • 20 cores
  • gcc 6.3
  • MKL 2016
  • PaRSEC-2.0-rc1
  • StarPU 1.2.1
  • CUDA 7.0
Dense Linear Algebra

DPLASMA = ScaLAPACK + runtime (PaRSEC)

DGEQRF performance strong scaling
Cray XT5 (Kraken) - N = M = 41,472

Systolic QR over PULSAR
Systolic QR over PaRSEC (2D)
DPLASMA HQR (best single tree)

LibSCI Scalapack

h stands for dynamic Hierarchical algorithms (a task can divide itself)
Relaxing constraints: Unhindered parallelism

• The only requirement is that upon a task completion the descendants are locally known
  • Information packed and propagated to participants where the descendent tasks are supposed to execute

• Uncountable DAGs
  • " %option nb_local_tasks_fn = ...”
  • PaRSEC provides support for global termination detection (or user provided)

• Add support for dynamic DAGs
  • Properties of the algorithm / tasks
    • "hash_fn = ...”
    • "find_deps_fn = ...”

• Allow dataflow specialization (RMA, datatype, displacement)
More dynamic applications

- use PAPI counters to estimate the imbalance
- reschedule the frontiers to balance the workload
Templated Task Graphs (TTG)

No synchronizations between the different algorithms, the data flows from one to another as soon as it becomes available.

Need for termination detection in the runtime

\[
\int_0^1 (g(x) + f(x)) \times g(x) - g(f(x)) \, dx
\]

double A(const double x) { return std::exp(-x * x); }
double B(const double x) { return std::exp(-x * x) * std::cos(x); }

auto p1 = make_project(&A, ctl, a, "project A");
auto p2 = make_project(&B, ctl, b, "project B");
auto d = make_diff(a, deriva, "dA/dx numeric");
auto b1 = make_binary_op(add, a, b, a_plus_b, "a+b");
auto b1 = make_binary_op(add, deriva, a_plus_b, b_minus_a, "b-a");
TESSE: Irregular tensor contraction

Accurate simulation of the electronic structure of molecules and solids using Coupled Cluster Singles and Doubles method (CCSD). Novel formulations replace the usual dense tensors with block-sparse and/or block-rank-sparse tensors increasing applicability from dozen to thousands of atoms.

\[ R_{ab}^{ij} = \sum_{cd} T_{cd}^{ij} G_{ab}^{cd} + \ldots, \]

Application dominated (90% of execution time) by 4-index block-distributed tensor contractions. These tensor operations can be mapped to matrix-matrix multiplications with irregular and imbalanced tiling.

![Tile Size Distribution for Irregular and Rectangular Problems](image)
for dealing with distributed environments. Legion describes heterogeneous architectures and have some nascent capabilities with the use of an external communication library. Communication needs to be explicitly described and performed. The OpenMP model is that distributed memory and internode communication in homogeneous, shared memory systems, and its use is the OpenMP model. OpenMP is widely used and supports homogeneous dataflow graphs. OpenMP is designed to relieve the master; however, the master-slave model may suffer. The master model allows nesting of tasks in individual nodes to improve scalability. The pruning phase limits potential scalability [12]. QUARK tasks that deliver or acquire input or output for the local tasks. QUARK reduces the set of locally executed tasks, and neighbor order to identify data movements between processes, before the peak for tile size of around 96x96.

2 streams are dedicated to memory transfer (up and down), we study the impact of the computing streams:

- 1 stream serializes calls, it will asymptotically reach peak;
- 2 streams already give enough performance by overlapping kernel calls with another kernel;
- 3 streams is enough in practice;
- 4+ might not [yet] be necessary.
Success story: Time to solution reduced by a factor of 3.5

Strong-scaling performance in the coupled-cluster doubles equation for (H2O)12 in aug-cc-pVDZ basis set.

The less appealing story is that despite the significant reduction in time to solution, we only reach 20% of the hardware peak for irregular problems when we are able to reach 60% regular GEMM.

At N = 64k each node holds 34GB of data, 3 times more than the GPU memory. Memory traffic between nodes (IB EDR 100Gbs) is the main culprit.
Example POTRI = POTRF + TRTRI + LAUUM

- 3 approaches:
  - **Fork/join**: complete POTRF before starting TRTRI
  - **Compiler-based**: give the three sequential algorithms to the Q2J compiler, and get a single PTG for POINV
  - **Runtime-based**: tell the runtime that after POTRF is done on a tile, TRTRI can start, and let the runtime compose
Interoperability with other programming paradigms

- With **OpenMP accelerator target**
  - Goal: improve PaRSEC portability by supporting OpenMP accelerators
  - GPU Engine modified to use OpenMP target data movement directives/functions (i.e. support for non-CUDA devices)
  - Data movement and management remains implicit from the end-user (simplified programming)
  - User provides an **OpenMP target task** that will be scheduled by PaRSEC
- With **Kokkos tasks**
  - User provides a Kokkos task that will be scheduled by PaRSEC
  - No tracking data dependencies at this point
  - Proof-of-concept demonstrator with **C to C++ translation** shim
- With **MPI programs**
  - PaRSEC Communication insulated from application MPI communication
  - MPI programs can enter/exit PaRSEC sections
  - PaRSEC does not consume resources when idle

PaRSEC can schedule data transfers to an OpenMP accelerator and schedule OpenMP target task.
ECP collaboration SLATE and Exa-PAPI

Providing support for SLATE C++ DSL/classes to unfold tasks over PaRSEC. Minimize the number of known tasks, explicit data collective patterns, batches executions, accelerator support.

Enhancing the runtime capabilities:
- mechanism for asynchronous completion of taskpools;
- multi-level task insertion to mitigate the overhead of dependencies resolution and enable the early detection of batched operations;
- API for explicit communication, type multicast;

- ECP Collaboration with Exa-PAPI: integration of PAPI-SDE interface into PaRSEC
- PaRSEC presents internal events as PAPI counters for external tools (e.g. tau, ScoreP)
- Counters exposed:
  - Number of pending tasks (in different schedulers), ready tasks, retired tasks
  - Memory usage by internal systems (communication, task, ...)
  - Extend the DSL to provide application/library level counters

- All counters are lock-free / wait-free / atomic-free and introduce measurable slowdown during the execution.

Energy consumption and performance during a dynamic execution where the number of computations resources is reduced

Evolution of some PaRSEC PAPI-SDE events during a POTRF factorization
The PaRSEC ecosystem

- Support for many different types of applications
  - Dense Linear Algebra: DPLASMA, MORSE/Chameleon
  - Sparse Linear Algebra: PaSTIX
  - Geophysics: Total - Elastodynamic Wave Propagation
  - Chemistry: NWChem Coupled Cluster, MADNESS, TiledArray
  - *: ScaLAPACK, MORSE/Chameleon, SLATE

- A set of tools to understand performance, profile and debug

- A resilient distributed heterogeneous moldable runtime

VampirTrace visualization of a POTRF execution in PaRSEC using the Open Trace Format traces (OTF2)
Conclusions

• Programming can be made easy(ier)
  • Portability: inherently take advantage of all hardware capabilities
  • Efficiency: deliver the best performance on several families of algorithms
  • Domain Specific Languages to facilitate development
  • Interoperability: data is the centric piece

• Build a scientific enabler allowing different communities to focus on different problems
  • Application developers on their algorithms
  • Language specialists on Domain Specific Languages
  • System developers on system issues
  • Compilers on optimizing the task code

• Interact with hardware designers to improve support for runtime needs
  • HiHAT: A New Way Forward
    for Hierarchical Heterogeneous Asynchronous Tasking