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PARALUTION - a Library for Iterative Sparse Methods on CPU and GPU

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Outline

Introduction and Motivation

PARALUTION Library

Solvers/Preconditioners

Integration with Application

Conclusion

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Introduction and Motivation

Multi/many-core systems are here

- CPUs, GPUs, Accelerators
- Trends - **more cores** CPU(16), MIC(60), GPU(2496)
- High performance, better performance/watt ratio

Scientific computing is expected to be

- **Fast** - use this new technology
- **Scalable** - use many cores (parallel)
- **Sustainable** over years

What is the Problem?

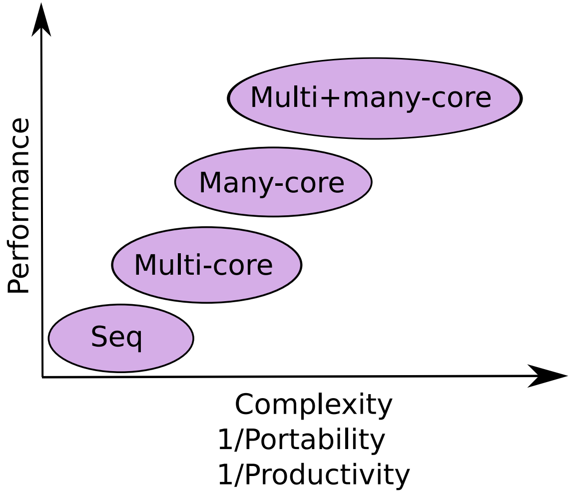
New algorithms

- High degree of parallelism
- Fine-grained parallelism
- Scalable = almost no communication

Software

- New programming models/languages
- Hardware-specific optimization techniques

Good Parallel Programming is HARD



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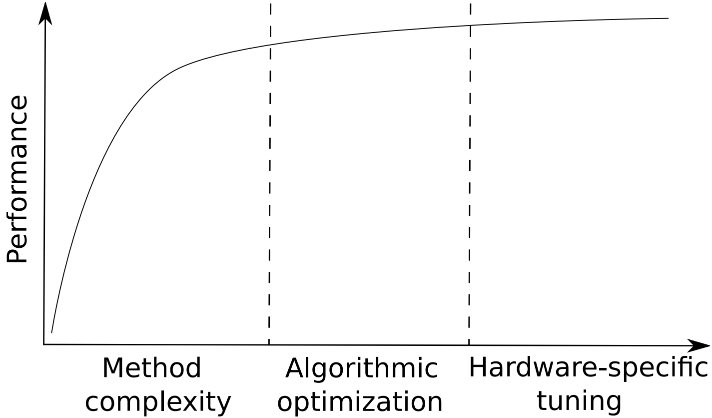
Methods are the MOST Important



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Goal

Create a library for iterative methods (linear and non-linear systems)!

Math

- Linear operators (sparse/dense matrices, stencils)
- Vector routines
- Extendable

Software

- Current multi/many-core dev, **new hardware**
- Portable code

PARALUTION

- Library for iterative sparse methods
- Targeting devices: CPUs + Accelerators (GPUs,...)
- Hardware abstraction
- No knowledge in OpenMP/CUDA/OpenCL required
- No special library/hardware required
- Portable results and code
- Run time type identification (RTTI)
- Easy to use
- Open source / GPL v3

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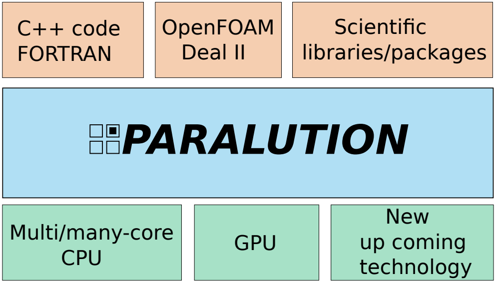
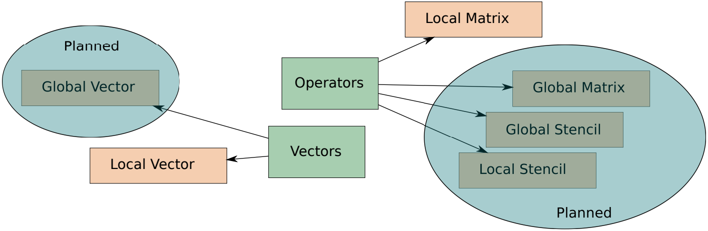
Middle-ware



Operators and Vectors



Local Vectors

- Init, Clear
- Standard vector routines
  - Dot product
  - Vector updates
  - Norm
  - ...
- Permutations
- Copy (sub-)vector to (sub-)vector
- I/O file
- Raw access via pointers

Local Matrices

- Init, Clear
- Formats – CSR, MCSR, COO, ELL, DIA, HYB, DENSE
- Conversion
- Matrix-vector multiplication
- Permutation
- Extract a sub-matrix
- I/O file
- Graph analyzer (CPU)
  - Multi-coloring
  - Maximal independent set
- Factorization
- Some wrapper to Intel/MKL

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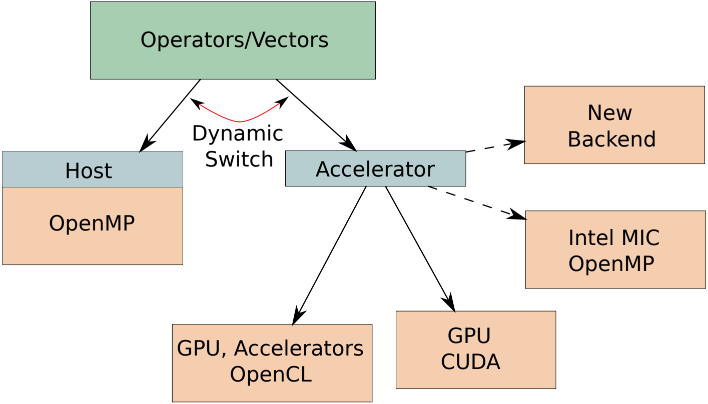
Operators and Vectors



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Source Example

```
LocalMatrix<ValueType> A;
LocalVector<ValueType> x, y ;

A.ReadFileMTX("my_matrix.mtx");
x.Allocate("vector1", mat.get_nrow());
y.Allocate("vector2", mat.get_ncol());

// y = A x
A.Apply(x, &y);

// Print the dot product of x and y
std::cout << x.Dot(y) << std::endl;
```

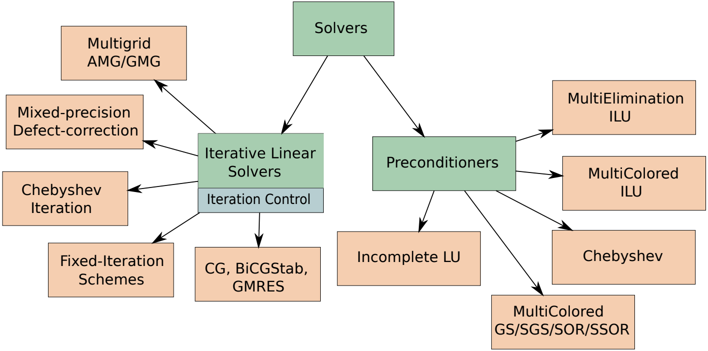
Source Example

```
LocalMatrix<ValueType> A;
LocalVector<ValueType> x, y ;

A.ReadFileMTX("my_matrix.mtx");
x.Allocate("vector1", mat.get_nrow());
y.Allocate("vector2", mat.get_ncol());

A.MoveToAccelerator();
x.MoveToAccelerator();
y.MoveToAccelerator();

A.Apply(x, &y);
std::cout << x.Dot(y) << std::endl;
```

Initialization/Shutdown

```
#include <paralution.hpp>

using namespace paralution;

int main(int argc, char* argv[]) {

  init_paralution();

  info_paralution();

  // ...

  stop_paralution();

}
```

Solvers


Solvers
Multigrid
AMG/GMG
Mixed-precision
Defect-correction
Iterative Linear
Solvers
Iteration Control
Chebyshev
Iteration
Fixed-Iteration
Schemes
CG, BiCGStab,
GMRES
Preconditioners
MultiElimination
ILU
MultiColored
ILU
Incomplete LU
Chebyshev
MultiColored
GS/SGS/SOR/SSOR

CG Solver

```
CG<LocalMatrix<ValueType>, LocalVector<ValueType>,
ValueType > ls;

ls.SetOperator(mat);

ls.Build();

ls.Solve(rhs, &x);
```

CG Solver

```
....

ls.MoveToAccelerator();
mat.MoveToAccelerator();
rhs.MoveToAccelerator();
x.MoveToAccelerator();

ls.Solve(rhs, &x);
```

PCG Solver

```
CG<LocalMatrix<ValueType>, LocalVector<ValueType>
ValueType > ls;
MultiColoredILU<LocalMatrix<ValueType>,
LocalVector<ValueType>, ValueType > p;

ls.SetOperator(mat);
ls.SetPreconditioner(p);

ls.Build();

ls.Solve(rhs, &x);
```

PCG Solver (same procedure)


```
....

ls.MoveToAccelerator();
mat.MoveToAccelerator();
rhs.MoveToAccelerator();
x.MoveToAccelerator();

ls.Solve(rhs, &x);
```

Design and Concepts

Hardware decision

- At run time
- No template parameter

MoveToHost/Accelerator

- All objects (matrices, vectors, solvers, preconditioners, etc)
- Always a CPU implementation

Template

- ValueType - float, double, int
- Solvers - Operator/Vector type

Design and Concepts

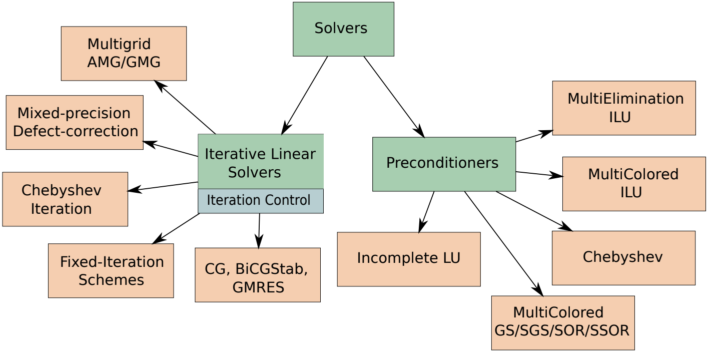
Functionality on the Accelerators

- Not all algorithms can be performed on the accelerator
- Ex: greedy multi-coloring, maximal independent set

The library has internal mechanism to check if a routine can be performed on the accelerator or not. If not the object is moved to the host and the routine is performed there.

- Always a CPU implementation
- Warning is printed if the object needs to be moved for the routine
- 100% portability of the code!

Iterative Linear Solvers



- Preconditioner = a solver
- Flexible design

Solver as Preconditioner

- Every solver can be used as a preconditioner
- Set a lower stopping criteria
- or/and Fixed number of iterations

Mostly used

- GS, SOR or SGS, SSOR
- GMG/AMG

PCG-AMG

```
CG<LocalMatrix<ValueType>,
LocalVector<ValueType>, ValueType > ls;

AMG<LocalMatrix<ValueType>,
LocalVector<ValueType>, ValueType > p;

p.InitMaxIter(2);

ls.SetPreconditioner(p);
ls.SetOperator(mat);

ls.Build();
```

Geometric Multigrid

Your application constructs

- Prolongation/Restriction operators or neighbor mapping vector

Pass it to PARALUTION and obtain

- Geometric Multigrid
- Interally constructed smoothers
- You can construct or pass the system matrices on all levels

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Plug-ins

Deal.II

- Export/Import vector/matrices
- Call PARALUTION solvers

OpenFOAM

- Compile PARALUTION with your application
- Configure the linear solver (txt file)

FORTRAN

- Pass matrix, vector
- Select a solver
- Obtain the solution vector

Advanced Integration

- Easy integration for any C++ code
- Can be hacked for everything (e.g. FORTRAN)

Avoid init times

- Do not init PARALUTION every time you call a solver
- Move the init in the beginning of your application

Raw data via pointers

- Create PARALUTION object via data pointers
- Obtain data via pointers from PARALUTION objs
- Host (OpenMP) and GPU (CUDA) backends
- No extra data copying

PARALUTION

Library for iterative sparse methods

- Various iterative solvers
- Various preconditioners

Backends

- OpenMP, CUDA, OpenCL
- Open for new hardware
- Portable results and code

General

- No special library/hardware required
- Easy to use
- Open source / GPL v3

PARALUTION - Doc

User Manual

- Installation
- Design
- Usage
- Examples

Doxygen

- Function descriptions
- Structure of the classes

Thank You for Your Attention

PARALUTION

www.paralution.com