LAtoolbox: A Multi-platform Sparse Linear Algebra Toolbox

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Engineering Mathematics and Computing Lab (EMCL)
The Shift towards Multicore/Manycore

Paradigm shift

- The paradigm shift towards manycore is well on the way
- But still many problems have to be overcome
  - Scalable algorithms and implementations, ubiquitous parallelism, programmers’ productivity, ...

- Many processors concepts have evolved (and some have gone)
  - x86, SPARC (2-12 cores)
  - NVIDIA / AMD GPUs (240 - 1536 cores)
  - Accelerated Processing Units
    (2-4 cores + 400 cores, hybrid CPU/GPU)
  - NVIDIA Denver (ARM-CPU + GPUs on a chip)
  - Cell, ClearSpeed (8+1, 92 cores)
  - Intel SCC, MIC (48, 32/80 cores)
  - Tile64, Epiphany (64, 64 - 4096 cores)

- Manycore trend: much higher core count, less complex cores
Manycore – Revolution or Evolution?

Manycore Devices
- High core count and incredible computing performance
- Fine-grained parallelism, stream processors + wide vector units
- Fast on-chip bandwidth, caches + local memory

Impact on the Software
- Without changing the software there will be no more speedups
- For performance benefits the mathematical models, algorithms, numerical schemes and programs need to be adapted, re-engineered and further developed
- New ways of parallel thinking required
The Programming Challenge

Zoo of languages and programming approaches

OpenMP, CUDA, OpenCL, OpenACC, ArBB, TBB, pthreads, UPC/PGAS, Cilk Plus, and many many more

Who can handle them all? Which is the best approach? We need some further abstractions!

Three main questions

- **Portability**: How portable is my program? (in terms of platforms and performance)
- **Flexibility**: Can I easily modify the software? (new modules, algorithms, platforms, functionality, ...)
- **Scalability**: How scalable is my algorithm/programming model? (ready for future platforms? ready for exascale?)
The Algorithmic Challenge

We have to rethink our methods and approaches!

Typical way of parallel thinking (?)

- Cluster-like problem decomposition with many fat nodes
  - Substructure problem into huge blocks (of same size)
  - Process blocks in parallel
  - Minimize communication between blocks
  - But typically: sequential processing on the block-level

New way of parallel thinking

- Decompose problem into blocks (of varying size)
  - There should be only a lower bound on the block size
- Process blocks in sequential order (or in parallel)
- But: use scalable parallelism on the block-level!
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Two Solution Approaches

We would like to show you two things:

I: How to build scalable and efficient algorithms
- How to re-arrange algorithms for scalable parallelism
- How to make them ready for GPUs and multicore CPUs
- How to keep mathematical quality and efficiency

II: How to build portable software (this talk!)
- Modular building of solver schemes
  - Single code base for GPUs, CPUs and other accelerators
  - Seamless integration of accelerators by unified interfaces
  - Choice of the platform can be taken at run time
- Highly optimized implementations
  - Transparent to the programmer/user
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I: How to build scalable and efficient algorithms

We have demonstrated new algorithms for parallel preconditioners on GPUs in Session S0289, Wednesday, May 16, 9:00am. Please check these slides for further details.

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HiFlow³ - Parallel Finite Element Software

- **Application Fields**: Numerical simulation in computational fluid dynamics, meteorology, medical engineering and energy research
- **Performance**: Scalability proven on huge clusters and GPU-accelerated systems
- **Flexibility**: Generic, modular and extensible software for multi-purpose simulation based on object-orientation in C++

\[ a(u,v) = (f,v) \]
HiFlow³ - Modules

- **Mesh**: Distributed and flexible mesh handling
- **FEM**: Finite element spaces
- **DoF**: Management of degrees of freedom
- **Integration routines**: Numerical integration and assembly routines
- **Linear algebra/solvers**: Multi-platform linear algebra and hardware-aware computing
Features of the LAtoolbox

Communication and computation layer of HiFlow$^3$

- Multi-platform parallelization (GPUs, multicore-CPU, accelerators, ...)
- Unified interfaces across platforms for all linear algebra operations and solvers
- Abstract data structures
- Platform-adapted library implementations chosen at run time
- No hardware knowledge required for building applications
- Minimal communication costs for intra-node data exchange

Solvers and preconditioners

- Iterative linear solvers: CG, (F)GMRES, geometric multigrid
- Newton-like solvers for nonlinear problems
- Parallel preconditioners for GPUs and CPUs
LAtoolbox - A Two Level Library

Parallelism is introduced on two levels:

- Coarse-grained parallelism by means of distributed grids and distributed data structures
- Fine-grained parallelism by means of platform-optimized linear algebra back-ends
Data Distribution and Communication
for Sparse Matrix-Vector Multiplication (SpMV)

Figure: Domain partitioning: Degrees of Freedom (DoF) of process $P_0$ are marked in green (interior DoF in diagonal block); the remaining DoF represent inter-process couplings for process $P_0$ (ghost DoF in off-diagonal block)
Data Distribution and Communication for Sparse Matrix-Vector Multiplication (cont.)

Sparse Matrix-Vector Multiplication:
- start asynchronous communication
- exchange ghost values
- \( y_{\text{int}} = A_{\text{diag}} \times_{\text{int}} \)
- synchronize communication
- \( y_{\text{int}} = y_{\text{int}} + A_{\text{offdiag}} \times_{\text{ghost}} \)
Advanced Features

**Advanced Features of the LAtoolbox**

- No irregular memory access over the PCIe bus by blocking techniques
- Raw access to the data is possible with explicit declaration of device-specific classes (e.g. for nested loops, irregular memory access, etc.)
- Possible mixture of different types of platforms in the cluster (e.g. nodes with and without GPUs)
ImpLAtoolbox - Sample Source Code 1/2

```cpp
lVector<double> *x, *y;

// initialize a vector on a specific platform
x = init_vector<double>(size, "vec x", platf, impl);

// clone y as x
y = x->CloneWithoutContent();

// Usage of BLAS 1
y->CopyFrom(*x); // y = x
x->Scale(5.0); // x = x * 5.0
y->Axpy(*x, 3.3); // y = y + 3.3*x
```
ImpLAtoolbox - Sample Source Code 2/2

```cpp
lMatrix<double> *mat, *mat_c;

// init empty matrix on a specific platform
mat = init_matrix<double>(0, 0, 0, "A", platf, impl, CSR);

// init CPU matrix
mat_c = init_matrix<double>(0, 0, 0, "A", CPU, OpenMP, CSR);
mat_c->ReadFile("matrix.mt");

// Copy the sparse structure
mat->CopyStructureFrom(*mat_c);

// Copy only the values of the matrix
mat->CopyFrom(*mat_c);

mat->VectorMult(*y, x); // x = mat*y
```
Example: Geometric Multigrid Solver

Model problem: \(-\Delta u = f\) in \(\Omega := (0, 1)^2 \setminus (0, 0.5)^2\)

Solve Poisson problem on the L-shaped domain
- Zero Dirichlet boundary conditions, i.e. \(u = 0\) on \(\partial \Omega\)
- Locally refined and statically adapted mesh
- Mixed finite elements: Q1 elements on quadrilaterals and P1 elements on triangles (avoiding hanging nodes)
- Problem size: 3,211,425 DoF

Matrix-based geometric multigrid solver
- Start with zero initial guess
- Relative residual of \(10^{-6}\) taken as stopping criterion
- Various parallel smoothers: Multi-colored Gauss-Seidel, power\((q)\)-pattern enhanced ILU\((p)\), FSAI
Solution in the L-shaped domain

Figure: Locally refined mesh for the L-shaped domain (left) and discrete solution of the Poisson problem for $f = 8\pi^2 \cos(2\pi x) \cos(2\pi y)$ (right).
Performance Data for the Multigrid Solver

Run time comparison for various smoothers and platforms

Platform: 2x Xeon quadcore CPU + Tesla S1070 4G memory
- Best multigrid solver with ILU(1,2) takes 2.75sec on the GPU
- Significantly faster than the best preconditioned CG solver (with ILU(1,2)) on the GPU with 158sec
Example: CG Solver for a 3D problem

3D-Neumann-Laplace problem

\[ -\Delta u = f, \quad \text{in } \Omega = [0, 1]^3 \]

\[ \frac{\partial u}{\partial n} = 0, \quad \text{on } \partial \Omega \]

Configuration of the conjugate gradient solver:

- Q1 finite elements
  - with 2.1 M degrees of freedom
- CG solver with absolute tolerance $10^{-14}$
- 510 iterations needed
- Double precision computations

Solution on a cluster with 16 GPUs:

- 8 nodes with two NVIDIA Tesla M1060 GPU each, 4G memory
- 20 Gbit/s Infiniband (small DDR switch)
Strong Scalability Results
for the 3D Neumann problem on a 16-GPU-cluster

Strong Scalability Test on a GPU Cluster

- Close to linear speedup for all GPU and CPU configurations
- Same source code for all setups
Summary

We have presented the easy-to-use Linear Algebra Toolbox

- Modular building of applications
- Same source code for all platforms
- No hardware knowledge required
- Can be compiled on all platforms
- Choice of the platform can be taken at run time

- Two-level parallelism with minimal communication costs
  - Distributed data across nodes
  - Linear algebra backends for GPUs, CPUs, and others
- We have demonstrated
  - Scalability – very good strong scalability for GPUs and CPUs
  - Portability – same source code for CPUs and GPUs
  - Flexibility – easy modifications of solvers and algorithms
  - Extensibility – add new backends for new platforms
Contact and Acknowledgements

Check our open-source software

The LAtoolbox is part of the HiFlow³ open source parallel finite element package with a rich suite of solvers. See http://www.hiflow3.org

Further information

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