HORIZON 2020 For Future Extreme Scale Systems

Bo Kågström, Lennart Edblom, Lars Karlsson; Laura Grigori; Iain Duff, Jonathan Hogg; Jack Dongarra, and Nick Higham Umeå University, Sweden; Inria Paris-Rocqueancourt, France; RAL—Science Technology Facilities Council, UK; and University of Manchester, UK

NLAFET—Aim and Main Research Objectives

Aim: Enable a radical improvement in the performance and scalability of a wide range of real-world

NLAFET Work Package Overview



WP1: Management and coordination

► WP5: Challenging applications—a selection

- applications relying on linear algebra software for future extreme-scale systems.
- Development of novel architecture-aware algorithms that expose as much parallelism as possible, exploit heterogeneity, avoid communication bottlenecks, respond to escalating fault rates, and help meet emerging power constraints
- Exploration of advanced scheduling strategies and runtime systems focusing on the extreme scale and strong scalability in multi/many-core and hybrid environments
- Design and evaluation of novel strategies and software support for both offline and online auto-tuning
- Results will appear in the open source NLAFET software library

WP2, WP3 and WP4 at a glance!

Linear Systems Solvers

iiii iii. iii:

- Hybrid BLAS
- Eigenvalue Problem Solvers
- Singular Value Decomposition Algorithms
- Lower Bounds on Communication for Sparse Matrices
- Direct Methods for (Near–)Symmetric Systems
- Direct Methods for Highly Unsymmetric Systems
- Hybrid Direct–Iterative Methods
- Computational Kernels for Preconditioned Iterative Methods
- Iterative Methods: use p vectors per it, nearest-neighbor comm
- Preconditioners: multi-level, comm. reducing

- Materials science, power systems, study of energy solutions, and data analysis in astrophysics
- WP7: Dissemination and community outreach Research and validation results; stakeholder communities

Research Focus—Critical set of fundamental LA operations

- ► WP2: Dense linear systems and eigenvalue problem solvers
- ► WP3: Direct solution of sparse linear systems
- ► WP4: Communication-optimal algorithms for iterative methods
- ► WP6: *Cross-cutting issues*
- WP2, WP3 and WP4: research into extreme-scale parallel algorithms WP6: research into methods for solving common cross-cutting issues

Avoid Communications—extreme-scale systems accentuate the need!

Algorithms have two costs (measured in time or energy):

- 1. Arithmetic (Flops)
- 2. Communication: moving data between
- Ievels of a memory hierarchy (sequential case)
- ▷ processors over a network (parallel case).

Running time of an algorithm involves three terms:
Flops * Time_per_flop



Gaps growing "exponential" with time Annual improvements

WP6: Cross-cutting issues and challenges!

Extreme-scale systems are hierarchical and heterogeneous in nature!

- Scheduling and Runtime Systems:
 - ▷ Task-graph-based multi-level scheduler for multi-level parallelism
 - Investigate user-guided schedulers: application-dependent balance between locality, concurrency, and scheduling overhead
 - ▷ Run-time system based on parallelizing critical tasks $(Ax = \lambda Bx)$
 - Address the thread-to-core mapping problem
- Auto-Tuning:
 - ▷ Off-line: tuning of critical numerical kernels across hybrid systems
 - Run-time: use feedback during and/or between executions on similar problems to tune in later stages of the algorithm
- ► Algorithm-Based Fault Tolerance:
- ▷ Explore new NLA methods of resilence and develop algorithms with these capabilities.

Generalized eigenvalue problem—need for autotuning!

Find pairs of eigenvalues λ and eigenvectors x s.t. $Ax = \lambda Bx$



Tunable parameters in state-of-the-art parallel QZ algorithm:

 $n_{\min 1}$ algorithm selection threshold $n_{\min 2}$ algorithm selection threshold $n_{\min 3}$ parallelization threshold

- # Words moved / Bandwidth
- ► # Messages * Latency

 $\mathsf{Time_per_flop} \ll 1 / \; \mathsf{Bandwidth} \ll \mathsf{Latency}$

I I			
Time per flop		Bandwidth	Latency
59%	Network	26%	15%
	DRAM	23%	5%

Goal: Redesign algorithms (or invent new) to avoid communication! *Attain lower bounds on communication if possible!*

Task-graph-based scheduling and run-time systems

- Express algorithmic dataflow, not explicit data movement
- Blocked Cholesky tasks: POTRF, TRSM, GEMM, SYRK
- PTG representation: symbolic, problem size independent



- Data flow based execution using PaRSEC (ICL-UTK)
- Assigns computations threads to cores; overlaps comm. & comp.
- Distributed dynamic scheduler based on NUMA nodes and data reuse



Figure 1: Cholesky PTG run by PaRSEC; 45% improvement



QR factorization Hessenberg-Triangular reduction QZ algorithm (generalized Schur decomposition)

 P_{AED} # processors for subproblems level-3 BLAS threshold MMULT cache-blocking block size NCB loop break threshold NIBBLE AED deflation window size $n_{\rm AED}$ #shifts per iteration $n_{
m shift}$ # deflation windows NUMWIN eigenvalues per window WINEIG WINSIZE window size WNEICR #eigenvalues moved together

Acknowledgments

NLAFET has received funding from the European Unions Horizon 2020 Research and Innovation Programme under Grant agreement No 671633.

Contact Information

NLAFET Coordinator: Prof. Bo Kågström (bokg@cs.umu.se)
 Dept. of Computing Science and HPC2N, Umeå University, Sweden
 Web-site: http://www.nlafet.eu
 Email: info@nlafet.eu

NLAFET Partners











The University of Manchester