Fast and Accurate Finite Element Multigrid Solvers for PDE Simulations on GPU Clusters

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fakultät für

Hardware isn't our friend any more

- Paradigm shift towards parallelism and heterogeneity
 - In a single chip: Multicores, GPUs, ...
 - In a workstation, cluster node, ...
 - In a big cluster, supercomputer, ...
- Data movement cost gets prohibitively expensive
- Technical reason: Power wall + memory wall + ILP wall = brick wall

Challenges in numerical HPC

- Existing codes don't run faster automatically any more
- Compilers can't solve these problems, libraries are limited
- Traditional numerics is often contrary to these hardware trends
- We (the numerics people) have to take action

FeatFlow-benchmark 1993–2008

- Set of Navier-Stokes solvers based on FEM-multigrid
- Sequential, reasonably fast machines (data courtesy J. Hron)



- Good: 80x faster in 16 years without changes to source code
- But: 1000x increase of peak performance in the same time
- Important: automatical speedup of conventional codes stagnates

Most important aspects of hardware paradigm shift

- Memory wall: moving data gets prohibitively expensive
- Different levels of parallelism

Conflicting situations

- Existing methods no longer hardware-compatible
- Neither want less numerical efficiency, nor less hardware efficiency

Challenge: new algorithmic way of thinking

Balance these conflicting goals

Consider short-term hardware details in actual implementations, but long-term hardware trends in the design of numerical schemes!

High-level take-away messages of this talk

- Things numerical analysts might want to know about hardware
- Thinking explicitly of data movement and in parallel is mandatory
- Unfortunately, there are many levels of parallism, each with its own communication characteristics
- Parallelism is (often) natural, we 'just' have to rediscover it
- Expressing parallelism in codes is a different story I won't talk about

Examples in my niche: Linear solvers for sparse systems

- Mixed precision iterative refinement techniques
- FEM-multigrid (geometric) for structured and unstructured grids
- Extracting fine-grained parallelism from inherently sequential ops
- Scale-out to (GPU-accelerated) clusters

Introduction

The Memory Wall Problem GPU Computing

Worst-case example: Vector addition

- Compute $\mathbf{c} = \mathbf{a} + \mathbf{b}$ for large N in double precision
- Arithmetic intensity: N flops for 3N memory operations
- My machine: 12 GFLOP/s and 10 GB/s peak

Consequences, back-of-an-envelope calculation

- To run at 12 GFLOP/s, we need $3/1 \cdot 8 \cdot 10^9 = 240 \text{ GB/s}$
- In other words, maximum performance is 1/24 of what we could do

This is not too far away from real-life

- SpMV reads all matrix entries once without reuse
- Data reuse only in coefficient vector
- Irregular access patterns and additional pressure (indirection vector)

The Memory Wall Problem

Moving data is almost prohibitively expensive

- Affects all levels of the memory hierarchy
 - Between cluster nodes (Infiniband)
 - From main memory to CPU
 - From CPU to GPU (PCIe)
 - Within chips (cache hierarchies)

Multicores make this worse

- Number of memory controllers does not scale with number of cores
- It can sometimes make sense to leave cores idle
- On-chip resources can be shared (common last-level cache)

Data locality is the only solution

- Maximise data reuse (manually or via choice of data structures)
- Maximise coherent access patterns for block-transfers and avoid jumping through memory

Raw marketing numbers

- $\blacksquare>2~{\rm TFLOP/s}$ peak floating point performance
- \blacksquare Lots of papers claim $> 100\times$ speedup

Looking more closely

- Single or double precision floating point (same precision on both devices)?
- Sequential CPU code vs. parallel GPU implementation?
- Standard operations' or many low-precision graphics constructs?

Reality

- GPUs are undoubtedly fast, but so are CPUs
- Quite often: CPU codes significantly less carefully tuned
- Anything between 5–30x speedup is realistic (and worth the effort)

GPUs and the Memory Wall Problem



GPUs are parallel wide-SIMD architectures

- General idea: Maximise throughput of many similar tasks rather than latency of individual tasks
- Note: CUDA-speak, but OpenCL essentially the same
- Independent *multiprocessors*, each with several ALUs
- One instruction scheduler per multiprocessor (SIMD)
- Shared memory and registers (16–48 kB per MP)
- Caches: 16 kB *texture cache* per 2–3 MPs, recently also 16–48 kB L1-cache per MP
- Hardware schedules threads to multiprocessors
- Threads may diverge at the cost of reduced throughput (SIMT-architecture)
- Restrictive rules for addressing memory from neighbouring threads
- Recently: global L2-cache

Kernel = blocks of threads

- Kernels are executed in blocks of threads
- Blocks are virtualised multiprocessors
- Hardware schedules which threads from which blocks are executed
- Threads in a block are executed in warps of size 32
- Hardware switches instantaneously to new warp in case of a stall (memory access etc.)
- Threads within each block may cooperate via shared memory
- Blocks cannot cooperate (implicit synchronisation at kernel scope)
- Kernels are launched asynchroneously
- Recently: Up to four smaller kernels active simultaneously for better ressource optimisation
- Shared memory and register file can be a resource bottleneck (limits the amount of simultaneously resident blocks)

CPU-GPU transfers

- Blocking and non-blocking transfers (of independent data)
- Streaming computations: Read A back, work on B and copy input data for C simultaneously

GPU is a co-processor

- CPU orchestrates computations on the GPU
- Example: iterative solver
 - CPU launches all kernels for one iteration
 - CPU blocks at last kernel that computes norm of residual
 - CPU performs convergence check
- Try to minimise CPU-GPU synchronisation
- GPUs and multicores: Use one orchestrating CPU core per GPU and use the remaining cores for CPU computations

Example #1:

Mixed Precision Iterative Refinement

Combatting the memory wall problem

Switching from double to single precision (DP \rightarrow SP)

- 2x effective memory bandwidth, 2x effective cache size
- At least 2x compute speed (often 4–12x)

Problem: Condition number

- For all problems in this talk: $\operatorname{cond}_2(\mathbf{A}) \sim h_{\min}^{-2}$
- Theory for linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$

$$\operatorname{cond}_{2}(\mathbf{A}) \sim 10^{s}; \frac{\|\mathbf{A} + \delta \mathbf{A}\|}{\|\mathbf{A}\|}, \frac{\|\mathbf{b} + \delta \mathbf{b}\|}{\|\mathbf{b}\|} \sim 10^{-k} (k > s) \quad \Rightarrow \quad \frac{\|\mathbf{x} + \delta \mathbf{x}\|}{\|\mathbf{x}\|} \sim 10^{s-k}$$

In our setting

Truncation error in 7–8th digit increased by s digits

Poisson problem on unit square

- Simple yet fundamental
- $\operatorname{cond}_2(\mathbf{A}) \approx 10^5$ for L = 10 (1M bilinear FE, regular grid)
- Condition number usually much higher: anisotropies in grid and operator

	Data+Comp.	in DP	Data in SP, Com	npute in DP	Data+Comp. in SP		
Level	L_2 Error	Red.	L_2 Error	Red.	L_2 Error	Red.	
5	1.1102363E-3	4.00	1.1102371E-3	4.00	1.1111655E-3	4.00	
6	2.7752805E-4	4.00	2.7756739E-4	4.00	2.8704684E-4	3.87	
7	6.9380072E-5	4.00	6.9419428E-5	4.00	1.2881795E-4	2.23	
8	1.7344901E-5	4.00	1.7384278E-5	3.99	4.2133101E-4	0.31	
9	4.3362353E-6	4.00	4.3757082E-6	3.97	2.1034461E-3	0.20	
10	1.0841285E-6	4.00	1.1239630E-6	3.89	8.8208778E-3	0.24	

 \Rightarrow Single precision insufficient for moderate problem sizes already

Iterative refinement

- Established algorithm to provably guarantee accuracy of computed results (within given precision)
 - High precision: $\mathbf{d} = \mathbf{b} \mathbf{A}\mathbf{x}$ (cheap)
 - Low precision: $\mathbf{c} = \mathbf{A}^{-1}\mathbf{d}$ (expensive)
 - \blacksquare High precision: $\mathbf{x} = \mathbf{x} + \mathbf{c}$ (cheap) and iterate (expensive?)
- Convergence to high precision accuracy if A 'not too ill-conditioned'
- Theory: Number of iterations $\approx f(\log(\text{cond}_2(\mathbf{A})), \log(\varepsilon_{\text{high}}/\varepsilon_{\text{low}}))$

New idea (Hardware-oriented numerics)

- Use this algorithm to improve time to solution and thus efficiency of linear system solves
- Goal: Result accuracy of high precision with speed of low precision floating point format

Refinement procedure not immediately applicable

- 'Exact' solution using 'sparse LU' techniques too expensive
- Convergence of iterative methods not guaranteed in single precision

Solution

Interpretation as a preconditioned mixed precision defect correction iteration

$$\mathbf{x}_{\mathsf{DP}}^{(k+1)} = \mathbf{x}_{\mathsf{DP}}^{(k)} + \mathbf{C}_{\mathsf{SP}}^{-1}(\mathbf{b}_{\mathsf{DP}} - \mathbf{A}_{\mathsf{DP}}\mathbf{x}_{\mathsf{DP}}^{(k)})$$

Preconditioner C_{SP} in single precision: 'Gain digit(s)' or 1-3 MG cycles instead of exact solution

Results (MG and Krylov for Poisson problem)

- Speedup at least 1.7x (often more) without loss in accuracy
- Asymptotic optimal speedup is 2x (bandwidth limited)

Example #2:

Grid- and Matrix Structures

Flexibility \leftrightarrow **Performance**

General sparce matrices (on unstructured grids)

- CSR (and variants): general data structure for arbitrary grids
- Maximum flexibility, but during SpMV
 - Indirect, irregular memory accesses
 - Index overhead reduces already low arithm. intensity further
- Performance depends on nonzero pattern (numbering of the grid points)

Structured matrices

- Example: structured grids, suitable numbering \Rightarrow band matrices
- Important: no stencils, fully variable coefficients
- direct regular memory accesses (fast), mesh-independent performance
- Structure exploitation in the design of MG components (later)

Combination of respective advantages

- Global macro-mesh: unstructured, flexible
- Iocal micro-meshes: structured (logical TP-structure), fast
- Important: structured ≠ cartesian meshes!
- Reduce numerical linear algebra to sequences of operations on structured data (maximise locality)
- Developed for larger clusters (later), but generally useful



Poisson on unstructured domain





- Nehalem vs. GT200, ≈ 2M bilinear FE, MG-JAC solver
- Unstructured formats highly numbering-dependent
- Multicore 2–3x over singlecore, GPU 8–12x over multicore
- Banded format (here: 8 'blocks') 2–3x faster than best unstructured layout and predictably on par with multicore

Example

Details: Unstructured grid multigrid

- Strategy: Reduce everything to SpMV
- Smoothing: Currently pursuing SPAI-like approaches
- Grid transfers
 - chose the standard Lagrange bases for two consecutively refined Q_k finite element spaces V_{2h} and V_h
 - function $u_{2h} \in V_{2h}$ can be interpolated in order to prolongate it

$$u_h := \sum_{i=1}^m x_i \cdot \varphi_h^{(i)}, \quad x_i := u_{2h}(\xi_h^{(i)})$$

• for the basis functions of V_{2h} and $u_{2h} = \sum_{j=1}^{n} y_j \cdot \varphi_{2h}^{(j)}$ with coefficient vector y, we can write the prolongation as

$$u_h := \sum_{i=1}^m x_i \cdot \varphi_h^{(i)}, \quad x := P_{2h}^h \cdot y$$

Example #3:

Parallelising Inherently Sequential Operations

Multigrid with strong smoothers Lots of parallelism available in inherently sequential operations Test case: anisotropic diffusion in generalised Poisson problem

- **•** $-div (\mathbf{G} \operatorname{grad} \mathbf{u}) = \mathbf{f}$ on unit square (one FEAST patch)
- $\blacksquare~{\bf G}={\bf I}:$ standard Poisson problem, ${\bf G}\neq {\bf I}:$ arbitrarily challenging
- Example: G introduces anisotropic diffusion along some vector field



Only multigrid with a strong smoother is competitive

Disclaimer: Not necessarily a good smoother, but a good didactical example.

Sequential algorithm

- Forward elimination, sequential dependencies between matrix rows
- Illustrative: coupling to the left and bottom

1st idea: classical wavefront-parallelisation (exact)



- Pro: always works to resolve explicit dependencies
- Con: irregular parallelism and access patterns, implementable?

2nd idea: decouple dependencies via multicolouring (inexact)

Jacobi (red) – coupling to left (green) – coupling to bottom (blue) – coupling to left and bottom (yellow)



Analysis

- Parallel efficiency: 4 sweeps with $\approx N/4$ parallel work each
- Regular data access, but checkerboard pattern challenging for SIMD/GPUs due to strided access
- Numerical efficiency: sequential coupling only in last sweep

3rd idea: multicolouring = renumbering

- After decoupling: 'standard' update (left+bottom) is suboptimal
- Does not include all already available results



- Recoupling: Jacobi (red) coupling to left and right (green) top and bottom (blue) – all 8 neighbours (yellow)
- More computations that standard decoupling
- Experiments: convergence rates of sequential variant recovered (in absence of preferred direction)

Tridiagonal Smoother (Line Relaxation)

Starting point

- Good for 'line-wise' anisotropies
- 'Alternating Direction Implicit (ADI)' technique alternates rows and columns
- CPU implementation: Thomas-Algorithm (inherently sequential)

	0	1	2	3	4	5	6	7	8	9	10	11
0	х	х				х	х					
1	х	х	х			х	х	х				
2		х	х	х			х	х	х			
3			х	х	х			х	х	х		
4				х	х				х	х		
5	х	х				х	х				х	х
6	х	х	х			х	х	х			х	X
7		х	х	х			х	х	х			X
8			х	х	х			х	х	х		2
9				х	х				х	х		
1	0					х	х				х	x
1	1					х	х	х			х	X
								S. 1	S			S. S.

Observations

- One independent tridiagonal system per mesh row
- \blacksquare \Rightarrow top-level parallelisation across mesh rows
- Implicit coupling: wavefront and colouring techniques not applicable

Cyclic reduction for tridiagonal systems

- Exact, stable (w/o pivoting) and cost-efficient
- Problem: classical formulation parallelises computation but not memory accesses on GPUs (bank conflicts in shared memory)
- Developed a better formulation, 2-4x faster
- Index nightmare, general idea: recursive padding between odd and even indices on all levels



Starting point

- CPU implementation: shift previous row to RHS and solve remaining tridiagonal system with Thomas-Algorithm
- Combined with ADI, this is the best general smoother (we know) for this matrix structure

	0	1	2	3	4	5	6	7	8	9	10	11
0	х	х				х	х					
1	х	х	х			х	х	х				
2		х	х	х			х	х	х			
3			х	х	х			х	х	х		
4				х	х				х	х		
5	х	х				х	х				х	х
6	х	х	х			х	х	х			х	Χ.,
7		х	х	х			х	х	х			X
8			х	х	х			х	х	х		2
9				х	х				х	х		
10						х	х				х	×
11						х	х	х			х	X

Observations and implementation

- Difference to tridiagonal solvers: mesh rows depend sequentially on each other
- Use colouring $(\#c \ge 2)$ to decouple the dependencies between rows (more colours = more similar to sequential variant)

Evaluation: Total Efficiency on CPU and GPU

Test problem: generalised Poisson with anisotropic diffusion

- Total efficiency: time per unknown per digit (μs)
- Mixed precision iterative refinement multigrid solver



Speedup GPU vs. CPU



Summary: smoother parallelisation

- Factor 10-30 (dep. on precision and smoother selection) speedup over already highly tuned CPU implementation
- Same functionality on CPU and GPU
- Balancing of numerical and parallel efficiency (hardware-oriented numerics)

Example #4:

Scalable Multigrid Solvers on Heterogeneous Clusters

Robust coarse-grained parallel ScaRC solvers GPU acceleration of CSM and CFD solvers

Goals

- Parallel efficiency: strong and weak scalability
- Numerical scalability, i.e. convergence rates independent of N
- Robust for different partitionings, anisotropies, etc.

Most important challenge

- Minimising communication between cluster nodes
- Concepts for strong smoothers so far not applicable (shared memory) due to high communication cost and synchronisation overhead
- Insufficient parallel work on coarse levels

Our approach: Scalable Recursive Clustering (ScaRC)

Under development at TU Dortmund

ScaRC for scalar systems

- Hybrid multilevel domain decomposition method
- Minimal overlap by extended Dirichlet BCs
- Inspired by parallel MG ('best of both worlds')
 - Multiplicative between levels, global coarse grid problem (MG-like)
 - Additive horizontally: block-Jacobi / Schwarz smoother (DD-like)
- Schwarz smoother encapsulates local irregularities
 - Robust and fast multigrid ('gain a digit'), strong smoothers
 - Maximum exploitation of local structure





Block-structured systems

- Guiding idea: tune scalar case once per architecture instead of over and over again per application
- Blocks correspond to scalar subequations, coupling via special preconditioners
- Block-wise treatment enables *multivariate ScaRC solvers*

Examples (2D case)

- Linearised elasticity with compressible material (2x2 blocks)
- Saddle point problems: Stokes (3x3 with zero blocks), elasticity with (nearly) incompressible material, Navier-Stokes with stabilisation (3x3 blocks)

$$\begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} = \mathbf{f}, \quad \begin{pmatrix} \mathbf{A}_{11} & \mathbf{0} & \mathbf{B}_1 \\ \mathbf{0} & \mathbf{A}_{22} & \mathbf{B}_2 \\ \mathbf{B}_1^T & \mathbf{B}_2^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \mathbf{p} \end{pmatrix} = \mathbf{f}, \quad \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} & \mathbf{B}_1 \\ \mathbf{A}_{21} & \mathbf{A}_{22} & \mathbf{B}_2 \\ \mathbf{B}_1^T & \mathbf{B}_2^T & \mathbf{C}_C \end{pmatrix} \begin{pmatrix} \mathbf{v}_1 \\ \mathbf{v}_2 \\ \mathbf{p} \end{pmatrix} = \mathbf{f}$$

 A_{11} and A_{22} correspond to scalar (elliptic) operators \Rightarrow Tuned linear algebra **and** tuned solvers

Concept: locality

- GPUs as accelerators of the most time-consuming component
- CPUs: outer MLDD solver
- No changes to applications!



Heterogeneous Accelerator Hardware

Poisson, FEASTSolid, FEASTFlow

Local

Smoother

(CPU, MG)

Ce ...

Backends

$$\begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix} = \mathbf{f}$$

$$\begin{pmatrix} (2\mu+\lambda)\partial_{xx}+\mu\partial_{yy}\\ (\mu+\lambda)\partial_{yx} & \mu\partial_x \end{pmatrix}$$

$$(\mu + \lambda)\partial_{xy}$$
$$\mu \partial_{xx} + (2\mu + \lambda)\partial_{yy}$$



Speedup Linearised Elasticity



- USC cluster in Los Alamos, 16 dualcore nodes (Opteron Santa Rosa, Quadro FX5600)
- Problem size 128 M DOF
- Dualcore 1.6x faster than singlecore (memory wall)
- GPU 2.6x faster than singlecore, 1.6x than dualcore

Speedup Analysis

Theoretical model of expected speedup

- Integration of GPUs increases resources
- Correct model: strong scaling within each node
- Acceleration potential of the elasticity solver: $R_{acc} = 2/3$ (remaining time in MPI and the outer solver)

$$\label{eq:max} {\rm I\hspace{-.1cm} S_{max}} = \frac{1}{1-R_{\rm acc}} \qquad \qquad S_{\rm model} = \frac{1}{(1-R_{\rm acc})+(R_{\rm acc}/S_{\rm local})}$$

This example



Simultaneous doubling of problem size and resources

- Left: Poisson, 160 dual Xeon / FX1400 nodes, max. 1.3 B DOF
- Right: Linearised elasticity, 64 nodes, max. 0.5 B DOF



Results

- No loss of weak scalability despite local acceleration
- 1.3 billion unknowns (no stencil!) on 160 GPUs in less than 50 s

Stationary Laminar Flow (Navier-Stokes)

$$\begin{pmatrix} \mathbf{A_{11}} & \mathbf{A_{12}} & \mathbf{B_1} \\ \mathbf{A_{21}} & \mathbf{A_{22}} & \mathbf{B_2} \\ \mathbf{B}_1^\mathsf{T} & \mathbf{B}_2^\mathsf{T} & \mathbf{C} \end{pmatrix} \begin{pmatrix} \mathbf{u_1} \\ \mathbf{u_2} \\ \mathbf{p} \end{pmatrix} = \begin{pmatrix} \mathbf{f_1} \\ \mathbf{f_2} \\ \mathbf{g} \end{pmatrix}$$

fixed point iteration

assemble linearised subproblems and solve with global BiCGStab (reduce initial residual by 1 digit) Block-Schurcomplement preconditioner

1) approx. solve for velocities with **global MG** (V1+0), additively smoothed by

for all Ω_i : solve for \mathbf{u}_1 with local MG

for all Ω_i : solve for \mathbf{u}_2 with local MG

2) update RHS:
$$\mathbf{d}_3 = -\mathbf{d}_3 + \mathbf{B}^{\mathsf{T}}(\mathbf{c}_1, \mathbf{c}_2)^{\mathsf{T}}$$

3) scale $\mathbf{c}_2 = (\mathbf{M}^{\mathsf{L}})^{-1}\mathbf{d}_2$

3) scale
$$\mathbf{c}_3 = (\mathbf{M}_p^2)^{-1} \mathbf{d}_3$$





magnitude of velocity + coarse grid

Stationary Laminar Flow (Navier-Stokes)

Solver configuration

- Driven cavity: Jacobi smoother sufficient
- Channel flow: ADI-TRIDI smoother required

Speedup analysis

	R_{i}	асс	S_{loc}	ocal	S_{total}	
	L9	L10	L9	L10	L9	L10
DC Re250	52%	62%	9.1x	24.5x	1.63x	2.71x
Channel flow	48%	_	12.5x	-	1.76x	-

Shift away from domination by linear solver (fraction of FE assembly and linear solver of total time, max. problem size)

DC F	Re250	Channel			
CPU	GPU	CPU	GPU		
12:88	31:67	38:59	68:28		

Summary and Conclusions

Hardware

- Paradigm shift: Heterogeneity, parallelism and specialisation
- Locality and parallelism on many levels
 - In one GPU (fine-granular)
 - In a compute node between heterogeneous resources (medium-granular)
 - In big clusters between compute nodes (coarse-granular)

Hardware-oriented numerics

- Design new numerical methods 'matching' the hardware
- Only way to achieve future-proof continuous scaling
- Four examples and approaches

Collaborative work with

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