Abstract



While we speculate what exascale hardware might look like, state-of-the-art numerics and our machines already diverge. Many new hardware generations or ingredients such as Skylake, manycores or Intel's Optane reduce caches per core, make more and more cores share one interconnect, or introduce additional memory levels with high latency. At the same time, many modern algorithmic paradigms such as multigrid, particle-in-cell or predictor-corrector schemes require irregular, non-continuous, repeated memory accesses, as well as non-trivial (meta) data assembly. As a result, data assembly, movement and exchange become constraining factors when we upscale or tune scientific software. We have to avoid them.

In this talk, we generalise the term communication-avoiding. We make it comprise (i) the reduction of data volume, (ii) the elimination of (meta) data generation, (iii) the reduction of data exchange frequency, (iv) the homogenisation of data access, (v) data access hiding and (vi) the localisation of data transfers. These criteria apply to both classic data exchange between compute nodes as well as data movements on the chip. Communication-avoiding then tackles the problematic divergence sketched above. While every code might require tailored solutions of its own to become communication-avoiding, we present some algorithmic techniques - for multigrid, particle-in-cell and predictor-corrector schemes - which seem to be generic patterns. They can inspire us how to write communication-avoiding software for various applications.



Stop talking to me - some communication-avoiding programming patterns

IPAM Workshop IV: New Architectures and Algorithms D.E. Charrier, B. Hazelwood, B. Reps, B. Verleye, M. Weinzierl, me and many others



Durham Cathedral, www.dur.ac.uk

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- 2

Why I love to think about algorithms and their implementation ...



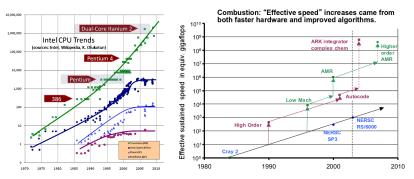
Chris Johnson (SCI, Utah):

Before the great discovery was the creation of a new tool!

("The Golden Age of Computing")

Performance increases—tool improves





H. Sutter: The Free Lunch Is Over: A Fundamental Turn Toward Concurrency in Software, 2005 (left)

D. Keyes: SCaLeS Report, Vol. 2, 2004 (right)

- Both sides improve our tools, yet are not orthogonal
- Better algorithms drive machine evolution(*)
- Changing machine characteristics require algorithmic rethinking
- Don't be naïve: hardware poses challenges to algorithms

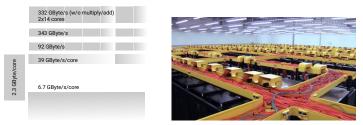
(*) If you believe in co-design:

https://www.hpcwire.com/2016/07/12/isc-workshop-tackles-co-developments-thorny-challenges

Tobias Weinzierl: Some communication-avoiding programming patterns— IPAM Workshop IV: New Architectures and Algorithms

This talk's challenge: data movements become showstopper





Left: Node of SuperMUC Phase 2; right: SuperMUC © IBM

Vertical New memory layers (Optane), new cache modi (Skylake)

Horizontal More cores per node, cache and network competition

The next big jumps on the algorithm side

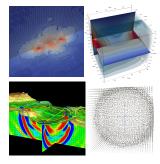
Remove data movement dependencies both intra-node & inter-node

- = Remove communication dependencies between computer components
- Communication-avoiding algorithms

but don't give up on the cool mathematics/algorithms

Outline





Motivation

Demonstrators

Communication-avoiding techniques

Avoid assembling data

Give up on task-traversal association

Prioritise communication tasks

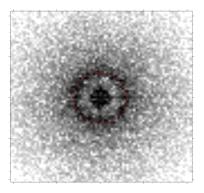
Predict synchronisation

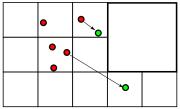
Drop the IEEE standard

Wrap-up

Particle-In-Cell (PIC)







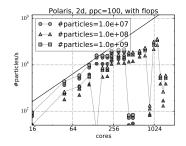
- 1. Solve PDE on (dynamically adaptive) mesh
- 2. Interpolate PDE solution onto particles
- 3. Move particles (suprathermal)
- 4. Restrict to PDE's rhs

Weinzierl, T., Verleye, B., Henri, P., Roose, D. Two Particle-in-Grid realizations on Spacetrees. Parallel Computing 52, 42–64, 2016. arXiv:1508.02435

Weinzierl, T. The Peano software—parallel, automaton-based, dynamically adaptive grid traversals. ACM Transaction on Mathematical Software (TOMS), 2nd revision. arXiv:1506.04496

Eckhardt, W., Glas, R., Korzh, D., Wallner, S., Weinzierl, T. (2016), On-the-fly memory compression for multibody algorithms, in Joubert, G.R., Leather, H., Parsons, M., Peters, F., Sawyer, M. eds, Advances in Parallel Computing 27: International Conference on Parallel Computing (ParCo) 2015. Edinburgh, Scotland, IOS Press, Amsterdam, 421–430 PIC





Likes

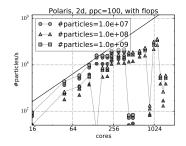
- Lagrangian plus Eulerian (best fit per subproblem)
- Break (Cartesian) mesh constraints
- Keep Cartesian efficiency for PDE

Flaws

- Particle updates/integrator cheap (arithmetic intensity)
- Maintain mapping
- Limited scalability
- Speed drops

PIC





Likes

- Lagrangian plus Eulerian (best fit per subproblem)
- Break (Cartesian) mesh constraints
- Keep Cartesian efficiency for PDE

Flaws

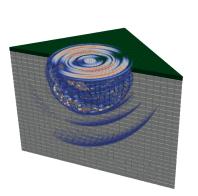
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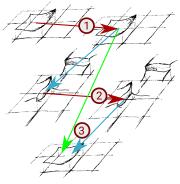
Speed drops result from latency-sensitiveness of bandwidth-bound particle movers

ADER-DG



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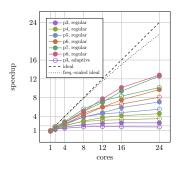


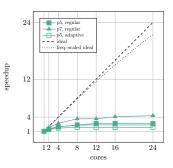
- 1. Predictor (non-linear iterate, implicit space-time)
- 2. Riemann
- 3. Corrector

Weinzierl, T. The Peano software—parallel, automaton-based, dynamically adaptive grid traversals. ACM Transaction on Mathematical Software (TOMS), 2nd revision. arXiv:1506.04496 Oharrier E. D., Weinzierl T. Stop talking to me – a communication-avoiding ADER-DG realisation. arXiv:1801.08682 Dumbser M., Fambri F., Tavelli M., Bader M., Weinzierl T. Efficient implementation of ADER discontinuous Galerkin schemes for a scalable hyperbolic PDE engine. arXiv:1808.03788

ADER-DG







Likes

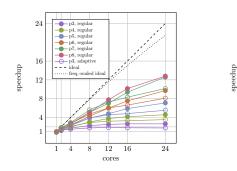
- Single shot (for large p)
- Localisation with expensive STP (arithmetic intensity)

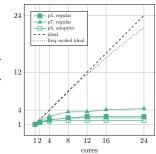
Flaws

- Three phases (synchronisation and data loads)
- Two phases extremely cheap (arithmetic intensity)

ADER-DG







Likes

- Single shot (for large p)
- Localisation with expensive STP (arithmetic intensity)

Flaws

- Three phases (synchronisation and data loads)
- Two phases extremely cheap (arithmetic intensity)

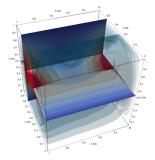
Obtained scalability suffers from one bandwidth-bound algorithm phases, time step size synchronisation and dynamic AMR's consistency constraints

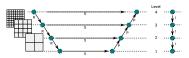
(Additive) Multigrid, BPX, ...

with complex shift



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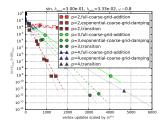


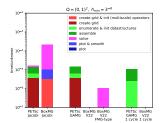
- 1. Solve on fine level
- 2. Solve correction on coarser level
- 3. Prolongate correction and sum up on fine level

Reps, B., Weinzierl, T. Complex additive geometric multilevel solvers for Helmholtz equations on spacetrees. ACM Transactions on Mathematical Software (TOMS), 44(1), 2:1–2:36, 2017. arXiv:1508.03954 Weinzierl, M., Weinzierl, T. Quasi-matrix-free hybrid multigrid on dynamically adaptive Cartesian grids, ACM Transactions on Mathematical Software (TOMS), 44(3), 32:1–32:44, 2018. arXiv:1607.00648

(Additive) Multigrid, BPX, ...







Likes

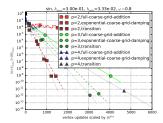
- Convergence speed (optimal)
- Conceptually simple improvements (smoother)

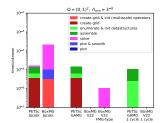
Flaws

- Touch unknowns multiple times
- Assembly time for (multiscale) operators
- Storage footprint of (multiscale) operators

(Additive) Multigrid, BPX, ...







Likes

- Convergence speed (optimal)
- Conceptually simple improvements (smoother)

Flaws

- Touch unknowns multiple times
- Assembly time for (multiscale) operators
- Storage footprint of (multiscale) operators

Suffers from low AI and high setup cost (assembly)



The root of all evil: We communicate.

Communication-avoiding (to me) is ...

- 1. reduction of data volume
- 2. elimination of (meta) data generation
- 3. reduction of data exchange frequency
- 4. homogenisation of data access
- 5. data access hiding
- 6. localisation of data transfer

Applies to node-to-node and CPU-to-memory.

This talk

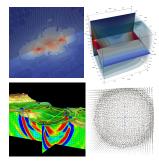


This talk: A tour de force through some communication avoiding techniques tailored to my demonstrators(*).

(*) With the potential to pay off in your projects, too.

Outline





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Communication-avoiding techniques Avoid assembling data

Give up on task-traversal association

Prioritise communication tasks

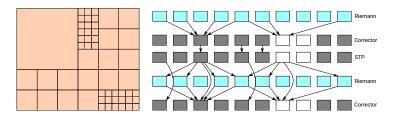
Predict synchronisation

Drop the IEEE standard

Wrap-up

HPC's lingua franca: Task graphs





ADER-DG

- ADER-DG describes a task pattern
- The mesh instantiates the task graph from this pattern
- Task graph conceptually simple
- ► Algorithm plus mesh plus graph ⇒ one item redundant

PIC and MG

Conceptually related

Task processing

Grid traversal = (partial) sweep over task graph

A plea against task graphs



Task assembly-free: Grid traversal spawns tasks, i.e. we use task parallelism without setting up a the task graph.

- Task pattern and instantiate rules exist already anyway
- Task assembly-free
- Mesh traversal acts as "scheduler"
- Avoid expensive assembly (graph changes each and every time step) (*)
- Eliminate meta data footprint (*)
- Best case: Throw away matrix data structures and matrix assembly, too (more on this later)

(*) I might be horribly wrong for static setups/meshes and more complicated algorithms

Why I am wrong-a double-edged sword



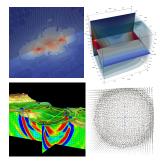
Task dependencies might require multiple grid sweeps

- Multiple data reads (no single-touch)
- Strong synchronisation between sweeps
- Temporary data
- Tiny tasks

Technique 1: Programming without (graph) assembly.

Outline





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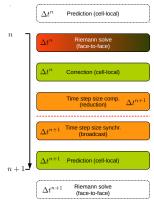
Wrap-up



Single touch implementation: A piece of data is read/written from main memory only once per iteration/time step.

Shifted tasking in ADER-DG





For the time being: assume Δt is known and there's no need to reduce it

Shifted algorithm:

- First read of face: trigger Riemann
- Enter cell: correct solution (all 2d faces are read already)
- Trigger subsequent STP immediately

Observations:

 Shifted execution model with two activities

(Riemann and one cell modification)

- ⇒ Task-fusion (incl. elimination of temporary memory)
- One time step per sweep
- \Rightarrow Amortised single-touch semantics
- Parallel traversal intermixes activities
- \Rightarrow Memory access homogenisation

Straightforward application to mat-vecs

- 1. Partial mat-vec computation: run over grid and contribute per-entity contribution
 - r = Ax
- 2. Apply action of r in next grid traversal

$$x \leftarrow x + \omega diag^{-1}(A)r$$

- 3. Immediately trigger follow-up computation
- \Rightarrow What happens in multiscale systems?



Pipelining in additive multigrid



1: function $TDADD(\ell)$ Shift evaluation by half a grid sweep $sc_{\ell} \leftarrow sc_{\ell} + Psc_{\ell-1}$ \triangleright Add coarse grid correction to sc_{ℓ} which 2: > so far, holds update resulting from a Jacobi smoothing step. 3. \triangleright Update *u* with update from $u_{\ell} \leftarrow u_{\ell} + sc_{\ell} + sf_{\ell}$ 4: previous line plus all updates done on finer grids. 5 $\hat{u} \leftarrow u_{\ell} - Pu_{\ell-1}$ Determine new hierarchical surplus. 6٠ if $\ell < \ell_{max}$ then 7: $TDADD(\ell + 1)$ ⊳ Go to next finer level. 8. end if 9: $r_{\ell} \leftarrow b_{\ell} - H_{\ell} u_{\ell}$ Determine residual and 10: $\hat{r}_{\ell} \leftarrow b_{\ell} - H_{\ell}\hat{u}_{\ell}$ bierarchical residual. 11. $sc_{\ell} \leftarrow \omega_{\ell} S(r_{\ell})$ Bookmark update due to a Jacobi 12: smoothing step for next traversal 13 14. if $\ell > \ell_{min}$ then $b_{\ell} \rightarrow R\hat{r}_{\ell}$ Determine right-hand side 15: 16. ▷ for multigrid correction. $sf_{\ell-1} \leftarrow I(sf_{\ell} + sc_{\ell})$ Inform other grids about update 17: b that is due in next traversal 18: > Update propagation aligns with traversal data flow 19 end if 20: 21. end function

Shifting summary



Lessons learned

- Suffered from tight association of grid traversals with algorithmic steps
- Don't eliminate temporary data on paper immediately (residual, unknown updates) but use them for pipelining
- Desynchronise grid entities (some already are ahead in the computation) anarchic mindset
- Not too difficult to prove correctness

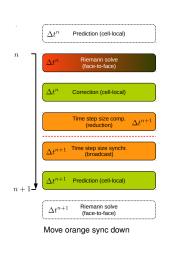
Open questions

- Increased memory footprint
- Stability(*)
- Causal dependencies

(*) Cmp. work by Vanroose et al. Likely not an issue here as only one step of pipelining.

Be optimistic and anarchic





- Intermix compute phases over different grid entities (data access homogenisation)
- Bring STP calculations forward
- Fuse correction with STP tasks
- Be optimistic (and eliminate synchronisation):
 - Work with estimate $\Delta t_{est}^{(n+1)}$
 - Determine $\Delta t_{adm}^{(n+1)}$ on-the-fly
 - ► If admissible $\Delta t_{adm}^{(n+1)} > \Delta t_{est}^{(n+1)}$ use $\Delta t_{est}^{(n+1)} \leftarrow 0.5(\Delta t_{adm}^{(n+1)} + \Delta t_{est}^{(n+1)})$
 - If $\Delta t_{adm}^{(n+1)} < \Delta t_{est}^{(n+1)}$ reset $\Delta t_{est}^{(n+1)} \leftarrow 0.9 \Delta t_{adm}^{(n+1)}$
- ⇒ AMR, time step decreases might make approach fall back to two-sweep paradigm
- \Rightarrow Does seem to happen negligible often
- PIC: Same time stepping mindset
- MG: Postpone analysis of termination criterion

Some metrics for ADER-DG



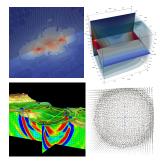
	1 core			12 cores			24 cores		
р	BW	Volume	Time	BW	Volume	Time	BW	Volume	Time
3	1,357.44	30.59	1.36	2,885.94	35.24	0.75	4,639.00	73.32	0.71
5	1,155.42	101.64	3.91	4,158.00	117.06	1.25	6,377.94	223.06	1.04
7	806.87	215.91	14.75	5,695.60	285.40	2.24	8,540.10	520.33	1.83
9	483.04	487.98	29.20	20,894.15	4,376.39	4.66	30,938.36	4,716.02	3.76
3	1,233.97	24.05	1.14	3,645.78	31.58	0.39	5,481.20	71.92	0.39
5	861.10	80.49	4.18	5,931.70	110.40	0.68	8,403.62	211.44	0.57
7	625.40	176.84	10.71	6,877.66	350.95	1.98	9,003.53	621.64	1.50
9	429.35	434.20	25.96	17,525.00	4,619.24	4.80	27,297.87	5,280.57	4.32

Performance counters for a 27 \times 27 \times 27 grid. Upper part: straightforward 3-step implementation. Lower part: fused approach. The bandwidth (BW) is given as MB/s, the volume (Vol.) transferred is given in GB, all timings are time per time step with [T] = s.

- the lower the AI the higher the reward
- optimistic assumption here failed in « 1%
- for very expensive STPs still burst of memory accesses (shift's homogenisation of memory accesses not sufficient)

Outline





Motivation

Demonstrators

Communication-avoiding techniques

Avoid assembling data

Give up on task-traversal association

Prioritise communication tasks

Predict synchronisation

Drop the IEEE standard

Wrap-up

Flaws in the task graph-free approach



Task assembly-free: Grid traversal spawns tasks, i.e. we use task parallelism without setting up a the task graph. \Rightarrow Traversal fires (and forgets) tasks.

Barely a new idea ignoring some showstoppers

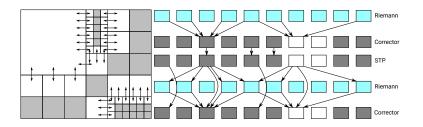
(on parallel computers)

In an ideal world, we would like to run through the whole grid with one large parallel for issuing face and cell operations, but

- cells along MPI boundaries have to be processed in order (MPI messages may not overtake)
- all cores might run Riemann (or any particular task type) concurrently (see experimental evidence for p = 9)
- dynamic AMR changes mesh between corrector and subsequent STP (memory allocation and initialisation/FV reruns synchronise code)
- AMR requires particular inter-grid transfer operator orders (multi-resolution data consistency)

Enclave tasking—inspired by Ghattas et al.





- ► Mark all cells along MPI boundary and resolution transitions ⇒ skeleton grid (those are involved in MPI and might refine/coarsen; this is an optimistic assumption)
- \Rightarrow reordering challenging
- Give up on idea to run Riemann solves parallel (at least on all of the cores)
- \Rightarrow bandwidth-bound

(cheap and skeleton operations done immediately and close-to sequentially)

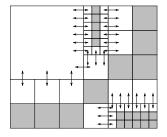
 Make remaining cells (enclaves) yield the scaling (job stealing brings in idling cores)

Prioritise tasks



Primary sweep:

- Per face
 - wait for adjacent STPs to finish (cmp. shifting)
 - Riemann solves
 - restrict image along resolution transitions
- Per cell
 - Corrector (bottom-up traversal)
 - Dynamic adaptivity, limiter reruns,
 - determine skeletons on-the-fly
- Spawn STP
 - on skeleton: high priority
 - on enclaves: low priority (background)



Prioritise tasks

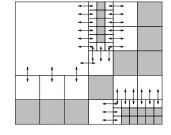


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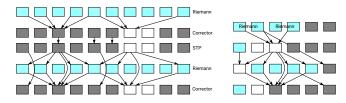
Secondary (partial) sweep:

- Ignore enclaves (partial traversal)
- Per skeleton cell: wait for STP
- Trigger MPI exchange
- Interpolate along AMR transitions for next Riemann solve





Enclave implications



- Low intensity tasks constantly trickle through system (homogenise arithmetic load/avoid memory access bursts)
- Coarsening & refinement accompanied by background/enclave STPs (avoid memory allocation and initialisation not throttling everybody else)
- STPs yielding MPI messages ran before majority of (enclave) tasks (more time to overlap messaging and processing)

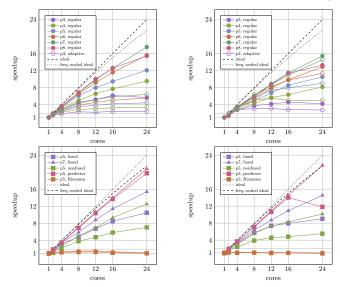
Implementation remarks:

- ► Skeleton traversal has highest priority ⇒ tweak TBB runtime
- ► Fuse multiple enclave tasks to reduce overhead ⇒ tweak TBB runtime



parallel for vs. enclaves

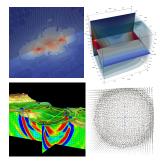
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Broadwell; top row: regular grid parallel for vs. tasks; bottom row: regular (left) vs. adaptive (right)

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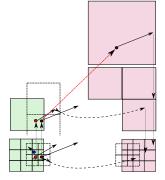
Predict synchronisation

Drop the IEEE standard

Wrap-up

The particle code





Single touch through shifts

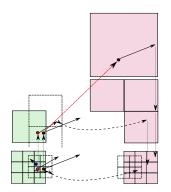
- Bookmark position update (do not apply)
- Apply position update as preamble to next step (first touch)
- Update grid-particle association in preamble, too
- ⇒ simple iff particles travel at most one cell per time step

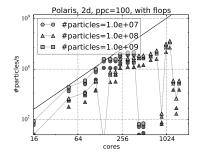
Data maintenance

- Use cascade of grids (octree)
- Particles on finest level for computation
- Otherwise on level such that they drift at most one level
- \Rightarrow lift-n-drop mechanism

The particle code





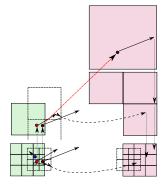


Horizontal data exchange

- Along multiscale domain boundaries (non-blocking MPI hiding behind computation)
- Very fast particles are lifted aggressively
- Non-neighbour MPI ranks involved (global sort)
- \Rightarrow Latency-sensitive

Predict data flow





Vertical data flow:

- ▶ Max velocity $v_{max}(c)$ per cell $c \in T$
- Extrapolate velocity updates (fine grid)
- Analysed tree grammar

$$v_{max}(c) = \begin{cases} max_{p \in c} |v(p)| & \text{for leaves} \\ max_{c'} v_{max}(c') & \text{otherwise} \\ \forall c' \sqsubseteq_{child of} c \end{cases}$$

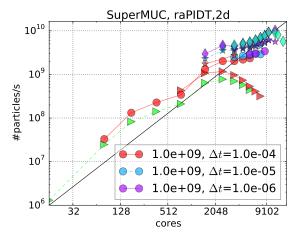
- Next traversal:
 - Particle p drops into domain

 $v_{max} \leftarrow max(v_{max}, |v(p)|)$

- v_{max} ≤ h/∆t: no tunnelling possible and likely not to happen either
- \Rightarrow skip reduction for these rank pairs
- Security factor for extrapolation

reduction-avoiding Particle-In-Tree





- ► Triangle: 2.0 · 10⁸ particles
- ▶ Diamond: 4.0 · 10⁹ particles
- ► Star: 1.0 · 10¹⁰ particles
- Colours encode time step sizes

Generic patterns



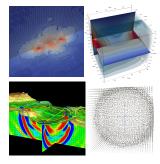
Communication graph replaces collective

Sparsify a priori (sparsity of communication graph anticipates particle positions and velocities)

 Similar pattern used to predict dynamic mesh refinement, wave fronts, time step size evolution

Outline





Motivation

Demonstrators

Communication-avoiding techniques

Avoid assembling data

Give up on task-traversal association

Prioritise communication tasks

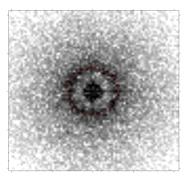
Predict synchronisation

Drop the IEEE standard

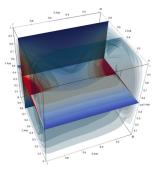
Wrap-up

Massive memory





- More particles more accurate physics
- Single-touch nice, but then homogeneously memory bound



- Pure geometric operators unstable
- Matrix-free not really an option

Information density



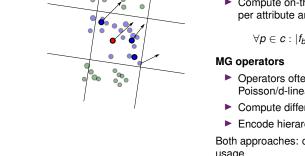
Particle sets

- Particles per cell carry similar values (often)
- Compute average attribute $\widetilde{A}(c)$ per cell
- Encode hierarchical $\hat{A}(p) = A(p) - \widetilde{A}(c)$ per cell
- Compute on-the-fly how many bytes per attribute are required such that

$$orall p \in {m c} : |f_{bpa}(\hat{A}(p)) - \hat{A}(p)| \leq \epsilon$$

- Operators often similar to Poisson/d-linear
- Compute difference to these stencils
- Encode hierarchical

Both approaches: convert back prior to next usage



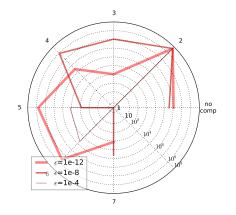
Reproducible science



```
void peano::heap::decompose( double value, char exponent[8], long int mantissa[8], double error[8] ) {
int shiftExponent = 6;
const long int sign = value < 0.0 ? -1 : 1;
if (sign < 0) {
  value = -value;
             integerExponent;
int
const double significand = std::frexp(value, &integerExponent);
for (int i=0; i<8; i++) {
  const double shiftMantissa = std::pow( 2.0, shiftExponent );
  exponent[i] = static_cast<char>( integerExponent-shiftExponent ):
  mantissa[i] = static_cast<long int>
    ( std::round(significand*shiftMantissa) );
  error[i] = std::abs( std::ldexp(mantissa[i].exponent[i]) - value ):
  std::bitset<64>* mantissaAsBitset =
    reinterpret_cast<std::bitset<64>*>(&(mantissa[i])):
  if (sign < 0) {
    mantissaAsBitset->flip((i+1)*8-1);
  shiftExponent+=8:
```

Forget IEEE

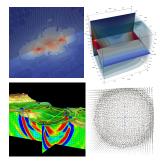




- Reduction of memory footprint
- "Almost" matrix-free for multigrid
- Generic observation: double values do often not carry enough significant bits compared to their neighbours/averages/recomputed data
- On-the-fly analysis: only compress where error is not too big

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My notion of "communication-avoiding"

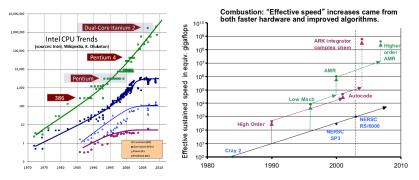


- 1. reduction of data volume (IEEE)
- 2. elimination of (meta) data generation (assembly)
- 3. reduction of data exchange frequency (shifts, fusion, prediction and batching)
- 4. homogenisation of data access (scheduling, shifts and enclaves)
- 5. data access hiding (enclaves)
- 6. localisation of data transfer (prediction)
- Generalised interpretation of "communication-avoiding"
- Applies to both message exchange and on-chip data access
- Might still be incomplete
- Requires us to rethink our implementations
- Benefits from generic implementation techniques
- Hunt for these techniques has just started

Message: It is more than posting sends and receives early. It is more than avoiding replicated messages. It is more than eliminating temporary data.



Context



H. Sutter: The Free Lunch Is Over: A Fundamental Turn Toward Concurrency in Software, 2005 (left) D. Keyes: SCaLeS Report, Vol. 2, 2004 (right)

- Some patterns have made/kicked off multifaceted impact:
 - Think multiresolution
- Time might be right for similar impact of communication avoiding techniques

Famous last words



Department of Computer Science

It is all open source (www.peano-framework.org or www.exahype.eu).

Support & Grants



- Peano (www.peano-framework.org) has been developed for more than 10 years under various grants made by Technische Universität München (TUM), KAUST, German Research Foundation (DFG), Durham University, and many more.
- ► ExaHyPE (www.exahype.eu) has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 671698.



The authors gratefully acknowledge the Gauss Centre for Supercomputing e.V. (www.gauss-centre.eu) for funding this project by providing computing time on the GCS Supercomputer SuperMUC at Leibniz Supercomputing Centre (LRZ, www.lrz.de).



Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities

Experiments were made possible through Durham's supercomputer Hamilton.



We appreciate early-adopters access to Intel Xeon Phi 7200 (codenamed KNL) family processors through the ► RSC Group.



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Some links



https://miscada.phyip3.dur.ac.uk



www.peano-framework.org and www.exahype.eu



dur.ac.uk/tobias.weinzierl