Challenges in Advanced Computing: Multi-this and Multi-that

Hans-Joachim Bungartz

TUM, Department of Informatics, Chair of Scientific Computing
Leibniz Supercomputing Centre of the Bavarian Academy of Sciences
Munich Centre of Advanced Computing

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Part I – General Remarks

Part II – Peano: Space-Filling Curves for PDE Solvers

Part III – Sparse Grids for High-Dimensional Numerics

Part I – General Remarks

Advanced Computing

The Software Challenge

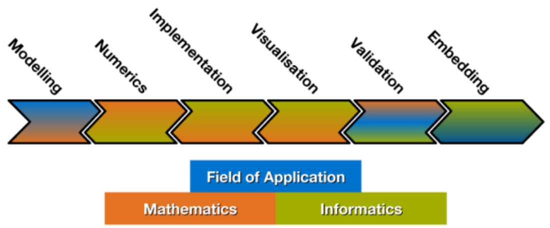
The Renaissance of Parallel Computing

Computational Science & Engineering (CSE)

➔ Key Technology for Science & Industry

High-Performance Computing (HPC)

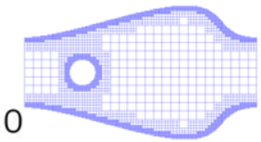
➔ Core Enabler for CSE



Mathematical model

$$
\begin{aligned}
\nabla \cdot \mathbf{u} &= 0 \\
\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\,\mathbf{u} + \frac{1}{\rho}\nabla p - \nu\,\Delta \mathbf{u} &= 0
\end{aligned}
$$

Discretization & solver



$$
\begin{aligned}
M\mathbf{u}_h &= 0 \\
A\dot{\mathbf{u}}_h + D\mathbf{u}_h + C(\mathbf{u}_h)\mathbf{u}_h - M^T p_h/\rho &= \mathbf{0}
\end{aligned}
$$

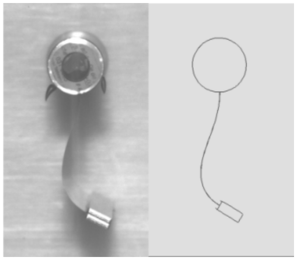
Impact of each step on all other steps!

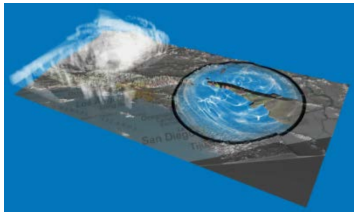
Hence #1: no pipeline any more, no cycle, but a complete graph

Hence #2: less space for single-field experts

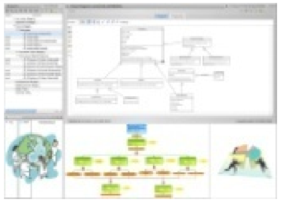
Parallel implementation, HPC

Validation





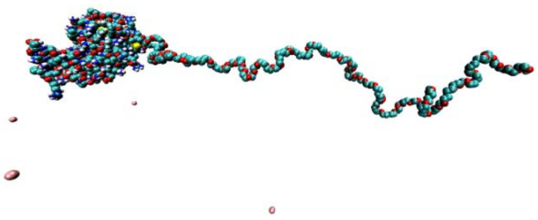
Software



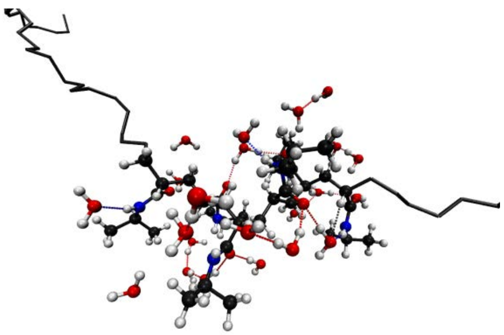
Insight, Design

Exploration

Atomistic Simulation of Protein Purification: State of the Art



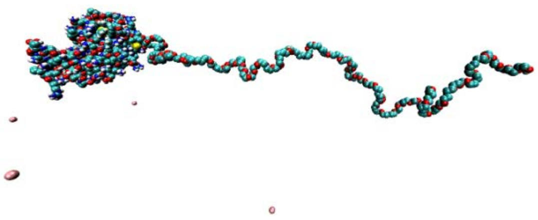
Polymer-modified protein in aqueous electrolyte solution



Solvent-hydrogel interactions

- Small scenarios (< 10^6 interaction sites)
- Short times (< 10^{-6} seconds)
- Moderately scaling codes (< 10^3 processes)
- Simulation times of weeks
- Benefit: qualitative insights

Atomistic Simulation of Protein Purification: State of the Art … and Vision Exascale



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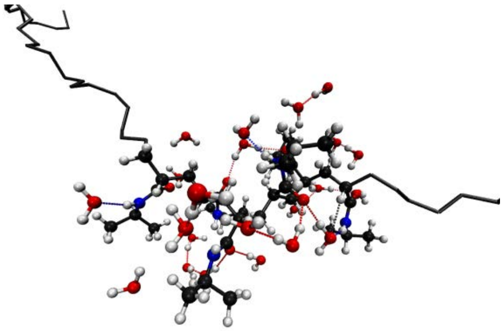

Solvent-hydrogel interactions

- Small scenarios (< 10^6 interaction sites)
- Large scenarios (> 10^{10} interaction sites)
- Short times (< 10^{-6} seconds)
- Long times (> 10^{-3} seconds)
- Moderately scaling codes (< 10^3 processes)
- Massively parallel codes (> 10^6 processes)
- Simulation times of weeks
- Response times of minutes
- Benefit: qualitative insights
- Quantitative insights and predictions

CSE/HPC Challenges

From data / images / numbers …
… to information / insight

From qualitative descriptions …
… to quantitative prediction

From counting operations …
… to energy awareness

From simulation …
… to optimisation

From sequential algorithm design …
… to massive parallelism

From parameter assumptions …
… to identification & estimation

From one-way batch jobs …
… to user interaction

Insight through computation & visualisation

From simple tools & codes …
… to 2x complex ones

From forward problems …
… to inverse problems

From heroic PhD codes …
… to large teams / SW

From deterministic models …
… to random & uncertainty

From hacker's delight …
… to complex workflows

From one (spatial/temporal) scale …
… to cascades of scales

From island fun …
… to embedding & integration

From single-physics problems …
… to coupled scenarios

From flat algorithms & data …
… to hierarchy

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Multi-scale

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CSE/HPC Challenges

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CSE/HPC Challenges

Multi-modal

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CSE/HPC Challenges

Multi-core

From data / images / numbers …
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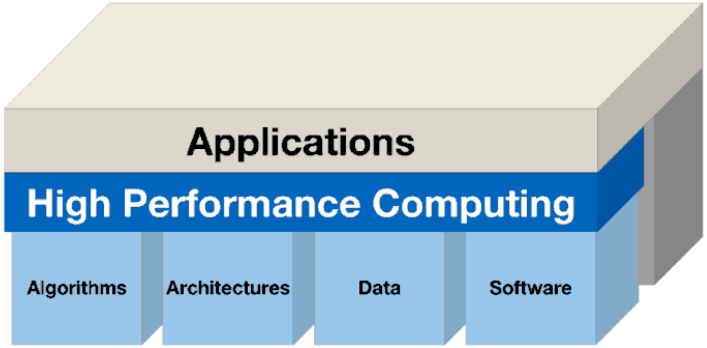
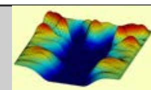
Beyond Moore: Enablers of Computing

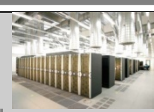


Computational Algorithms



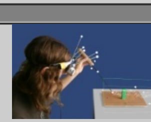
- Computational statistics
- Differential equations & multi-physics problems

Parallel Architectures



- {Homo/hetero}geneous multicore architectures
- Parallelisation support & programming models

Data Engineering / Exploration



- Database technology & data mining
- Visual analytics

In general: increasing relevance of informatics
[languages, compilers, tools, (par)prog paradigms, data exploration, visualization, algorithms and data structures (hierarchy & recursion), hardware-aware algorithmics, HW-SW-co-design, software engineering ...]

In particular: increasing relevance of software issues

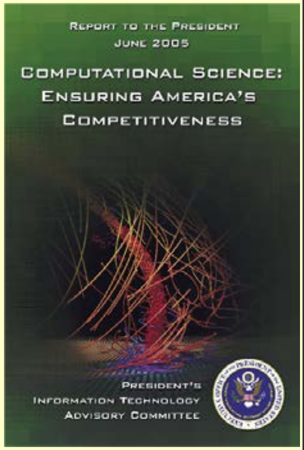
- Classical **software engineering**
  - specification
  - modular design
  - configuration management
  - documentation and sustainability
  - ...
- Algorithmic **verification and validation**
- Adaptive software **lifecycle management**
- Handling PSE & simulation **workflows**
- Systematic **testing**
- **Languages, compilers, runtime systems**
- **User interfaces**
- **Tool development** & professional **tool support**
- **Performance** tuning (esp. parallel)

Software in CSE/HPC – State of the Art

"Today's CSE ecosystem is unbalanced, with a software base that is inadequate to keep pace with and support evolving HW and application needs."

"The crisis in CSE software is multifaceted and remediation will be difficult. The crisis stems from years of inadequate investments, a lack of useful tools, a near-absence of widely accepted standards and best practices, …, and a simple lack of perseverance by the community. This indictment is broad and deep, covering applications, programming models and tools, data analysis and visualization tools, and middleware."

PITAC report 2005



"The field has reached a threshold at which better organization becomes crucial. New methods of verifying and validating complex codes are mandatory if CSE is to fulfil its promise …."

"Verification, validation, and quality management, we found, are all crucial to the success of a large-scale code-writing project."

Post and Votta, *Computational Science Demands a New Paradigm*, Physics Today, 2005

"In many domains software engineering quality management processes like CMMI and ISO 9000 have been successful, but apparently less so in CSE, especially in HPC-related applications."

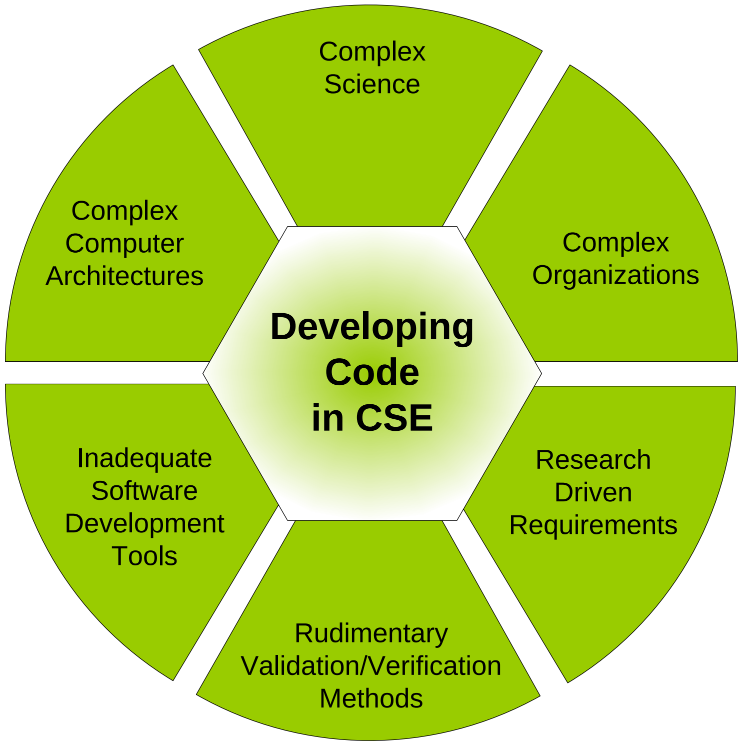
R. Kendall, *Advanced Computing Focus Day*, Informatik 2008, München

Studies on CSE-Related SW Development in the US (DoD, DoE – ASCI and successors; study from 2004)

Development team size (median): 6	increasing
Code size (median): 300 k LoC	increasing
Number of users (median): 25	stable
Code project age (median): 17.5 years	increasing
Presence of Fortran: 58% (24% F77, 34% F90/95)	decreasing

Source: Kendall, Post, et al.

Some Observations on SW Development in CSE

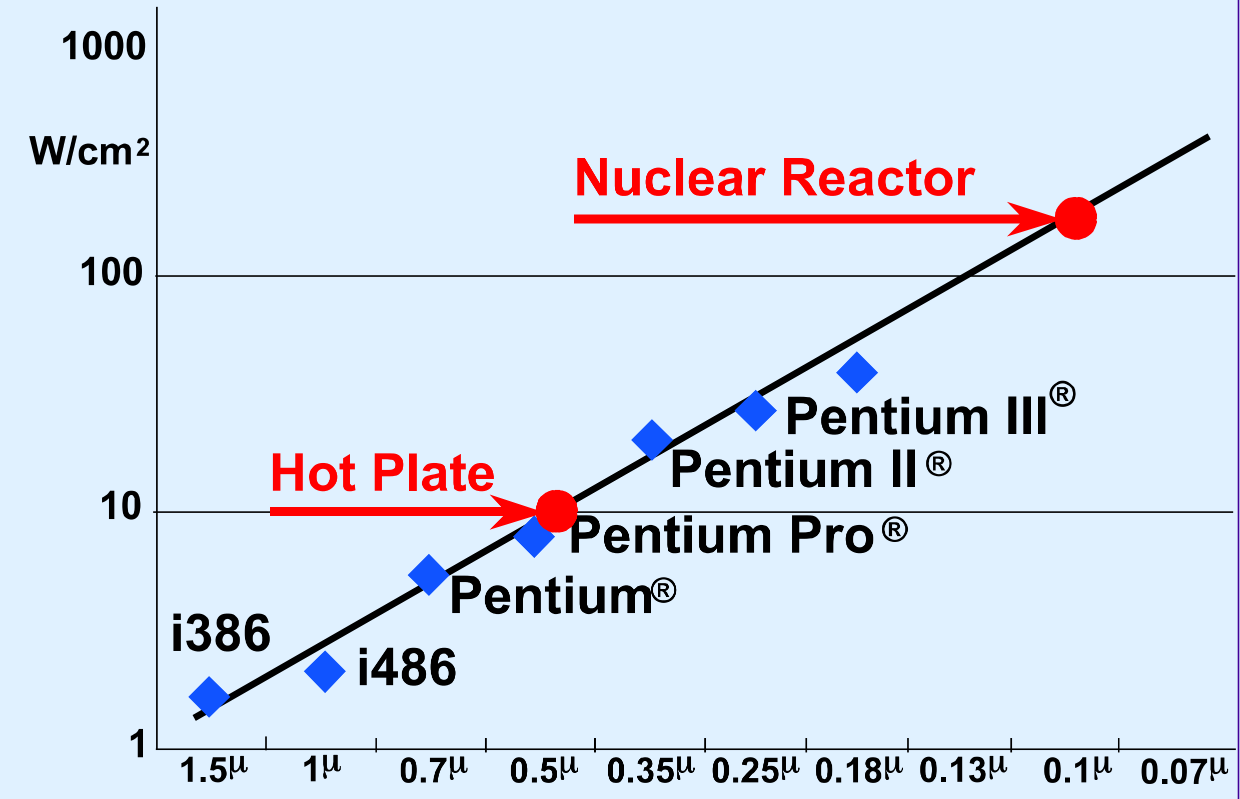


"Software development is the principal bottleneck in CSE" (R. Kendall)

Roadblocks:

- Most developers are domain scientists and engineers, not computer scientists
- Typical priority: science >> code performance >> software quality
- Intellectual level assigned:
  models >> algorithms >> programs
- No "software engineering mainstreaming": design, process models, workflow models, …
- No "team understanding": co-operative work, trans-disciplinary, project management, …
- Instead, still the lonely heroes with their heroic codes (and sometimes accumulated heroism)
- No systematic testing culture
- No formal support – verification
- No best practices
- Many groups working on PSE – in general with limited success

Energy Density – the Fundamental Problem



Source: Fred Pollack, Intel. New Microprocessor Challenges in the Coming Generations of CMOS Technologies, Micro32

We‘re no longer getting faster – we‘re getting more!

Traditional Sources of Performance Improvement are Flat-Lining

- **New Constraints**
  - 15 years of *exponential* clock rate growth has ended
- **But Moore’s Law continues!**
  - How do we use all of those transistors to keep performance increasing at historical rates?
  - Industry Response: #cores per chip doubles every 18 months *instead* of clock frequency!

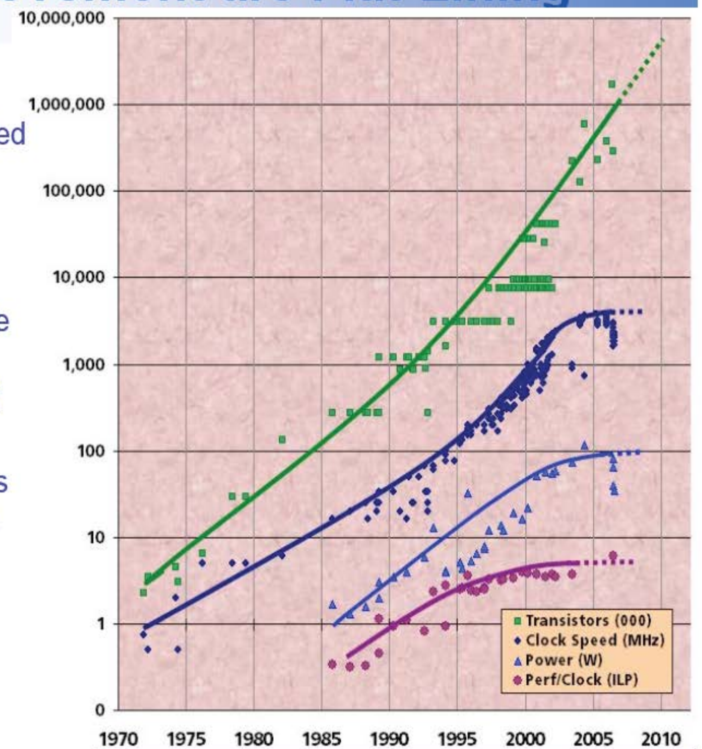
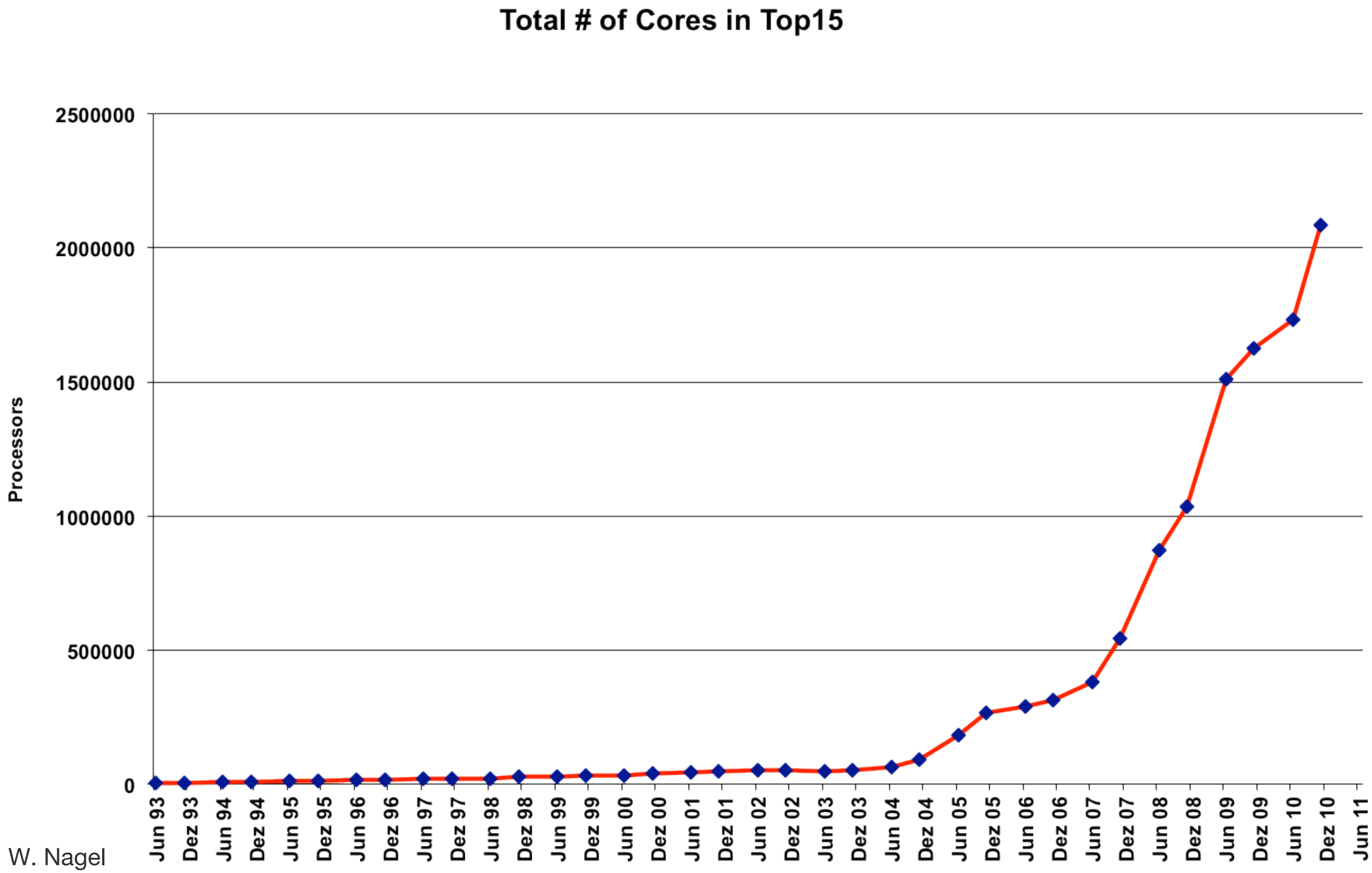


Figure courtesy of Kunle Olukotun, Lance Hammond, Herb Sutter, and Burton Smith

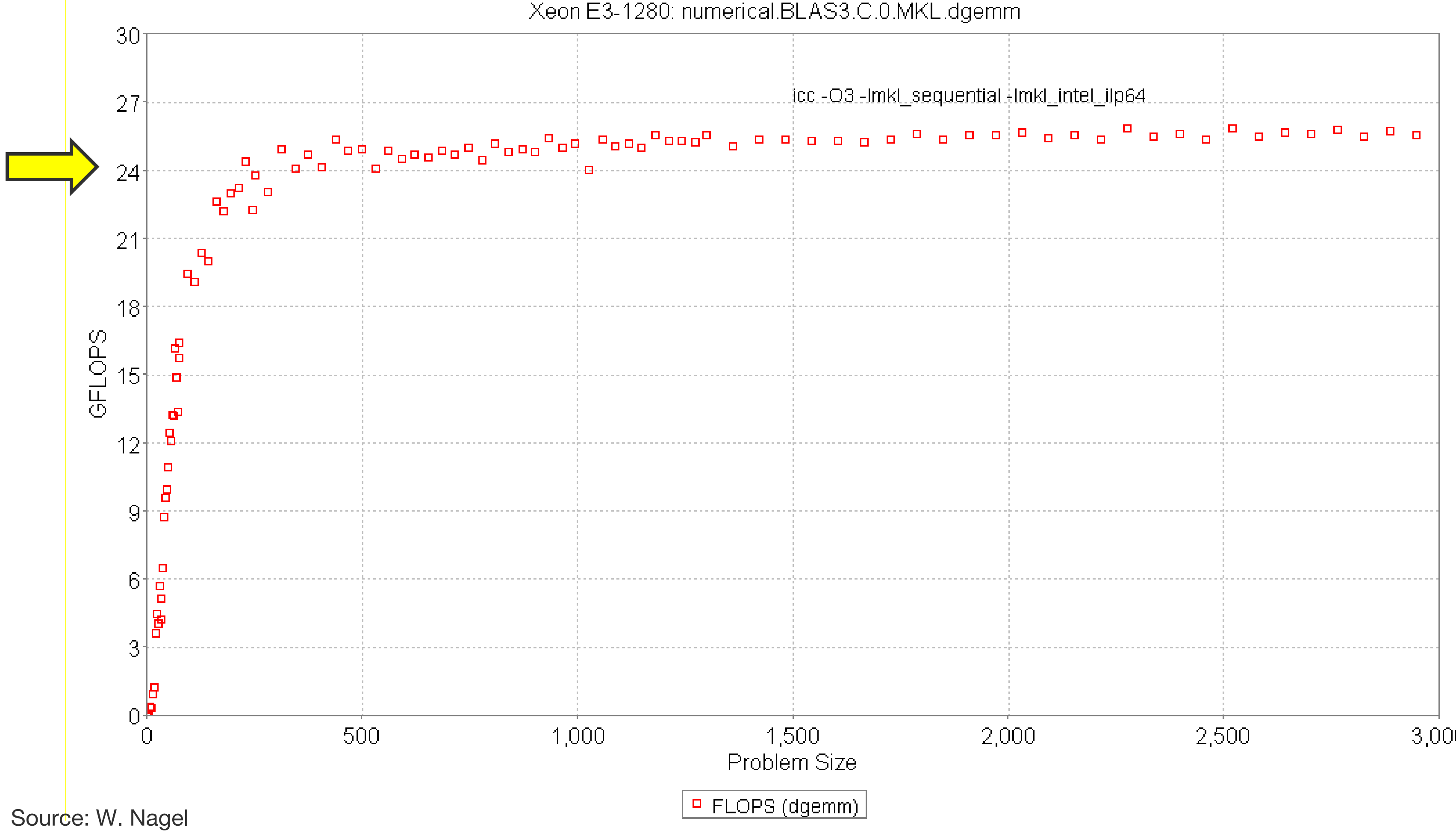
Office of Science
U.S. DEPARTMENT OF ENERGY

Increase of Numbers of Cores



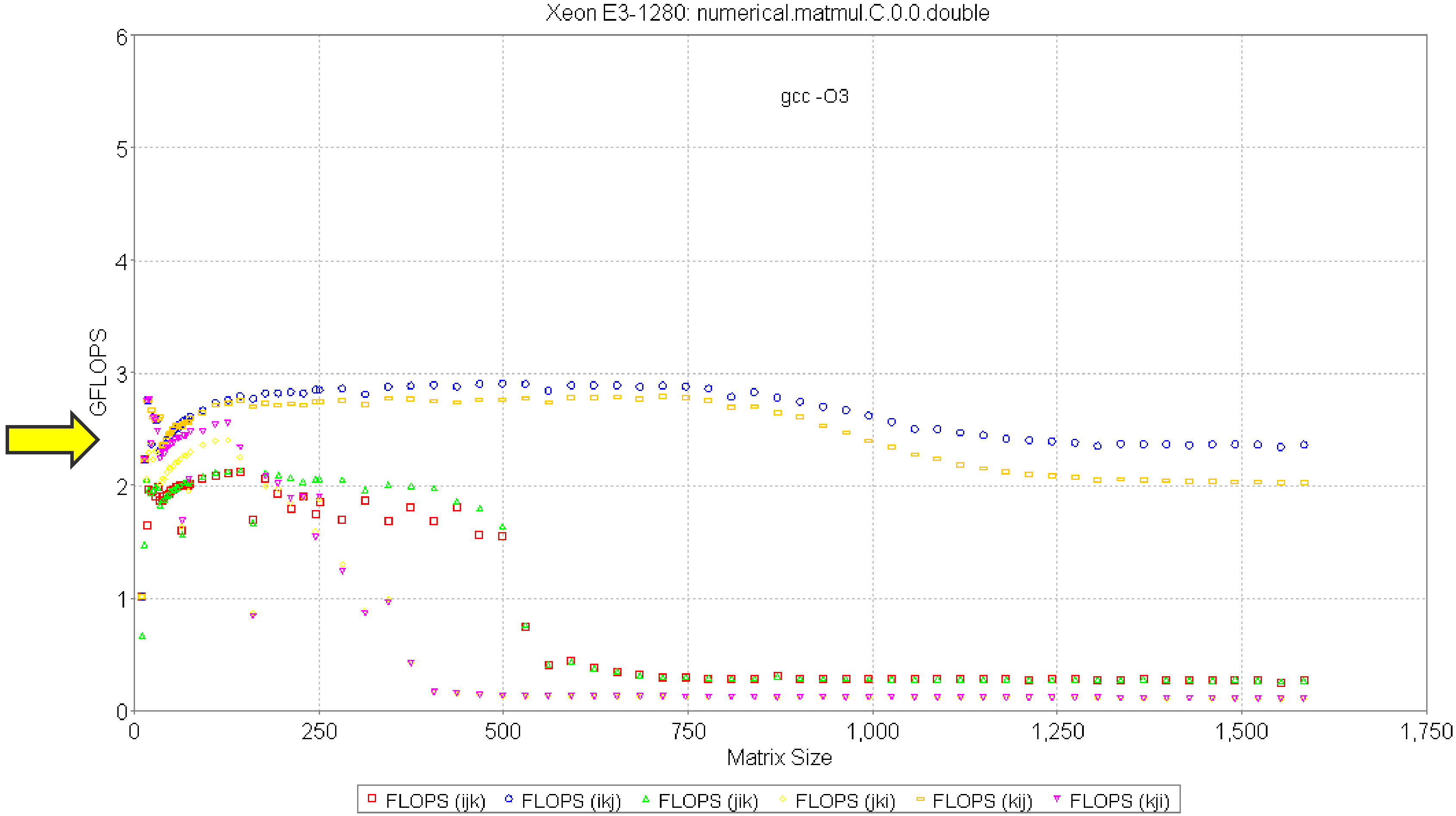
Source: W. Nagel

Sandy Bridge MatMult – Best Ingredients



Source: W. Nagel

Sandy Bridge MatMult – Straightforward (C, gcc, …)

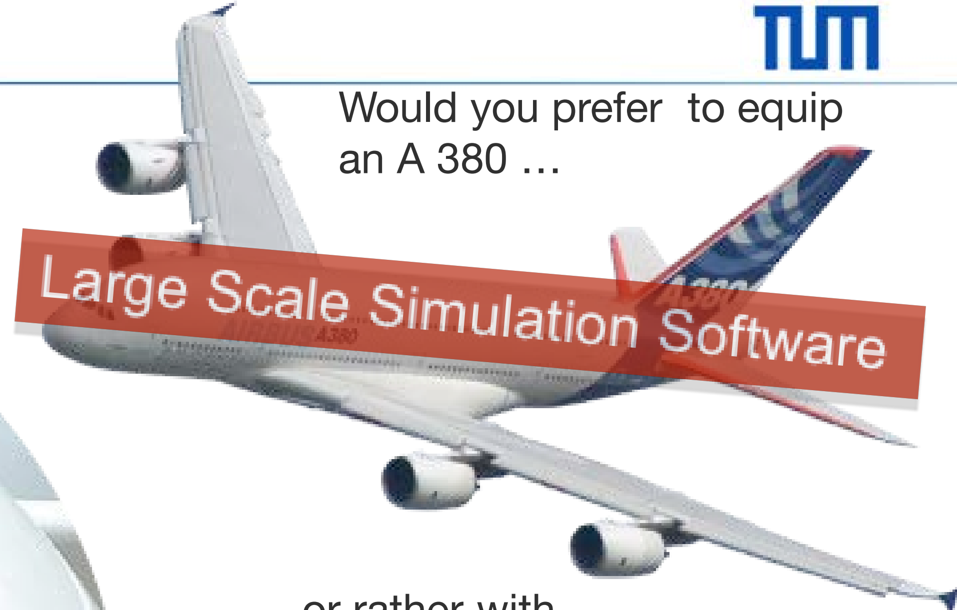


Source: W. Nagel

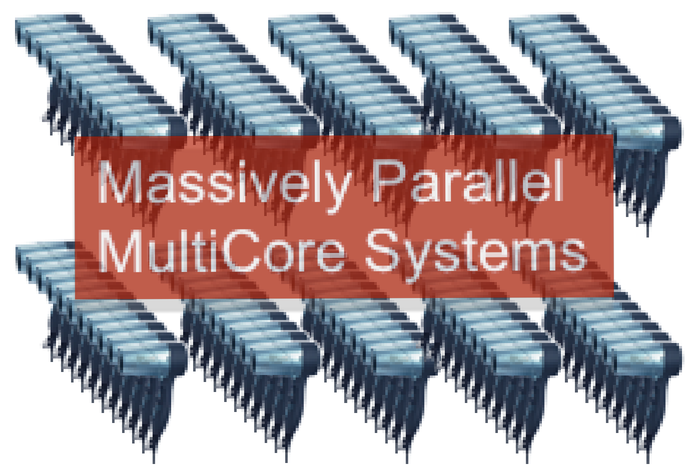
Why All New?

… with 4 strong jet engines …

Would you prefer to equip an A 380 …



… or rather with 100,000 hair dryers??



Source: U. Rüde

Part II – Peano: Space-Filling Curves for PDE Solvers

The Scope of Space-Filling Curves

The Peano Project

Applications

[not discussed here]

Algorithmic Challenges – and Changes

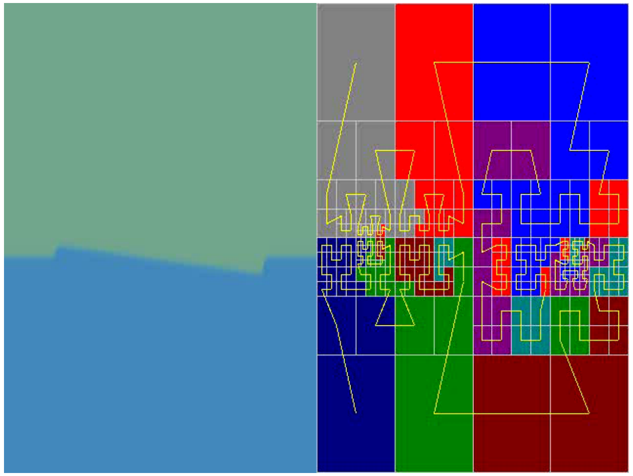
- Tackling the "memory wall":
  - cache-awareness via sophisticated traversal strategies
  - cache-oblivious vs. cache-conscious
- Tackling on-chip parallelism (multi-core):
  - multi-threading, fine-grain parallelism
  - no more "sequential kernel"
  - non-standard hardware: accelerators, such as GPGPU, (Cell), FPGA (?)
- Tackling scalability: hybrid concepts, sophisticated & cheap load balancing
  - heterogeneous scenarios (non-standard geometry, multi-level schemes, …) require dynamic load balancing
  - intra- and inter-system (from hybrid systems to the Grid)

Annual gain in last years: (avg.)
- CPU performance: 60%
- memory bandwidth: 23%
- memory latency: 5%

➔ A promising paradigm: space-filling curves

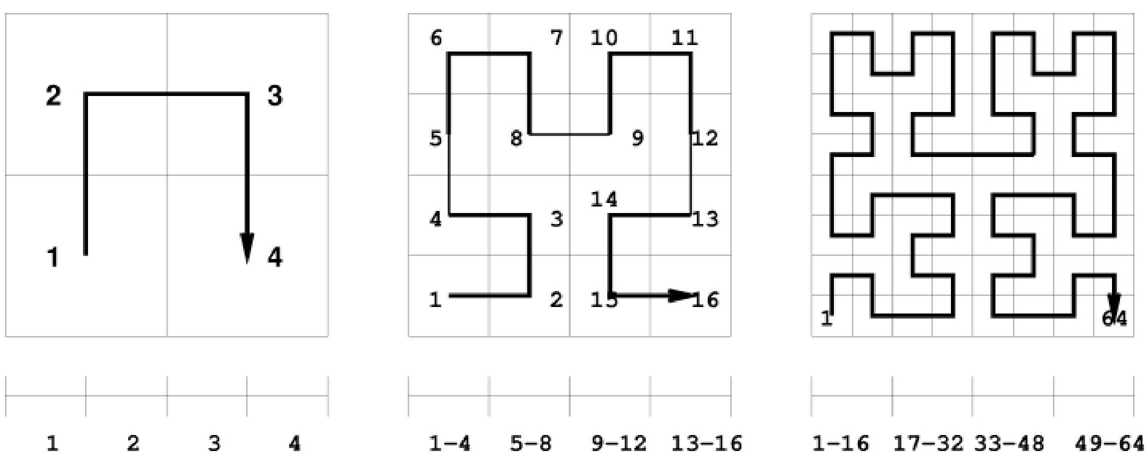
[SFC: continuous and surjective mapping from unit interval onto unit square/cube]

- **Lebesgue**: the classical one (Morton, Z, octree)
- **Hilbert**: the most famous one
- **Peano**: our favourite for Cartesian grids
- **Sierpinski**: the newcomer for triangles & Co.



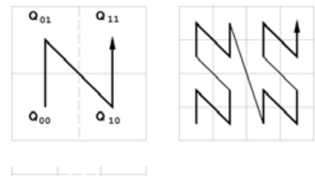
What is a Space-Filling Curve?

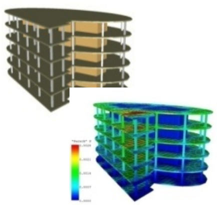
- **curve**: continuous mapping from the unit interval to a 2D/3D/… reference domain (unit square, unit cube, potato, ...)
- **space-filling**: mapping is surjective *[rather strange that this works ... bijective won't]*
- **purpose**: serialize high-dim data *[facilitates data organization, access, queries, partitioning, ...]*
- **construction**: recursive process, following *inclusion* and *neighbourhood*
- **example**: Hilbert curve

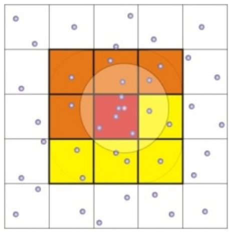


Overview of Space-Filling Curves *(there are more!!)*

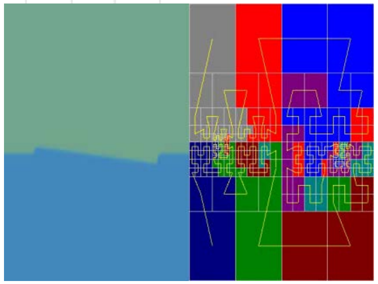
Lebesgue
- organizing simulation tasks



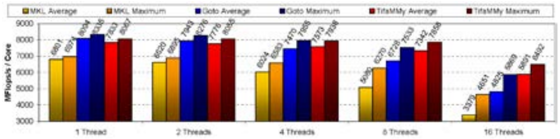


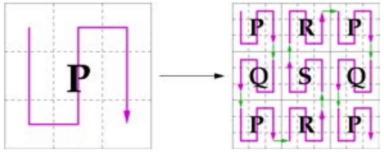


Hilbert
- dynamic load balancing

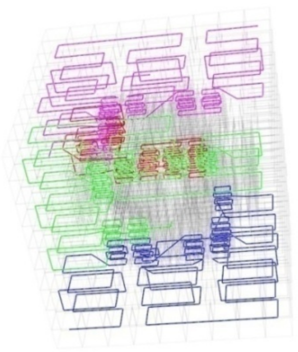


Peano
- matrix-matrix multiplication

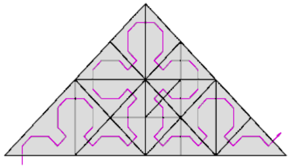


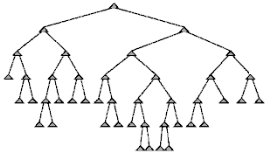


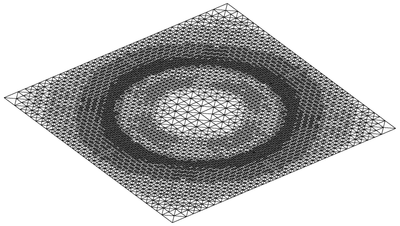
Peano
- PDE solvers



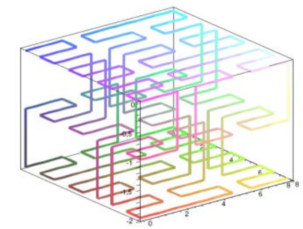
Sierpinski
- Tsunami simulation





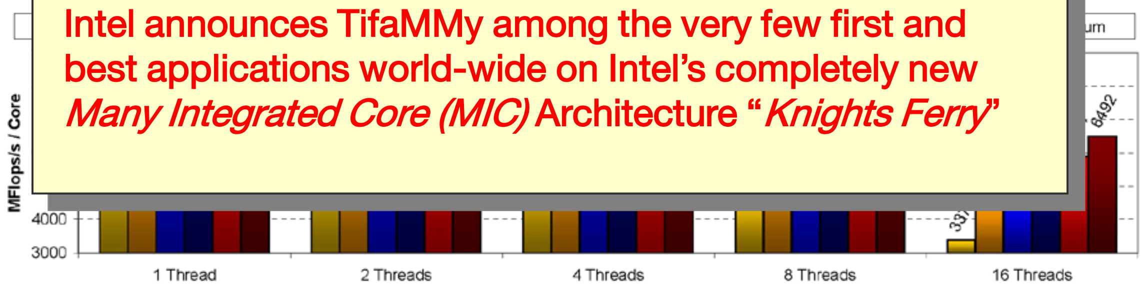


SFC #1a – Peano: Numerical Linear Algebra

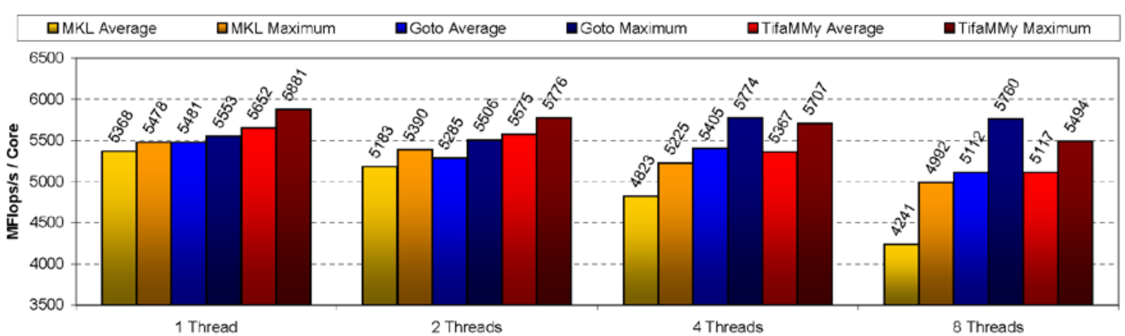


TifaMMy – cache-efficient matrix multiplication

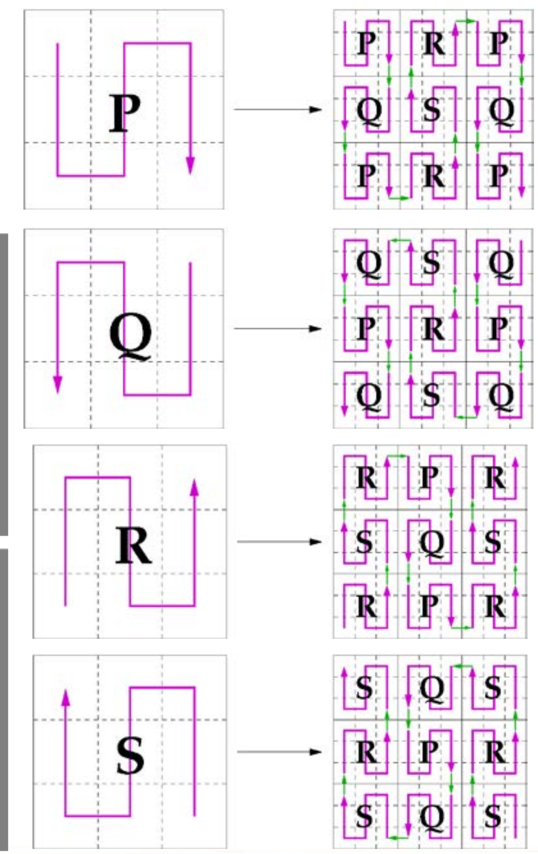
- Peano-based traversal with high locality (dense or sparse matrices)
- block-structured data structure and algorithm
- parallel @ multicore: HW-conscious kernel, OpenMP
- parallel @ clusters: distributed caches, MPI
- application: quantum control (states via matrices)
- **LATEST NEWS from ISC '11, Hamburg, June 20, 2011: Intel announces TifaMMy among the very few first and best applications world-wide on Intel's completely new *Many Integrated Core (MIC)* Architecture "*Knights Ferry*"**



Xeon (4 x quad)



AMD (2 x quad)



SFC #1b – Peano: Iterative Solvers for PDE

PDE solvers:

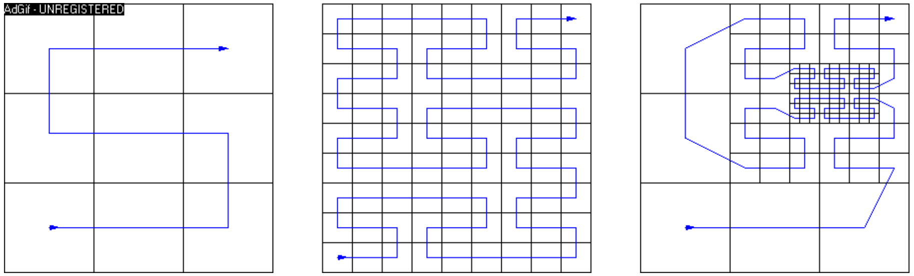
- high cache efficiency (>99.9% L2), low memory requirement (10^9 d.o.f. on 1 GB RAM!)
- easy access to parallelisation and dynamic load distribution
- no restrictions w.r.t. adaptivity
- full multigrid potential

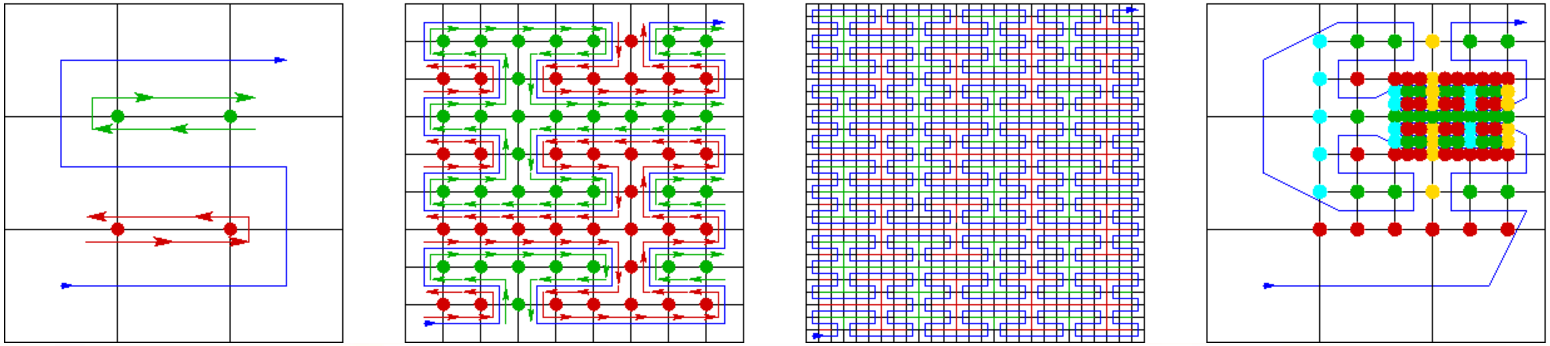
Organisation:

- Recursive partitioning

Ordering:

- based on space-filling (Peano) curves
- for geometry representation, iterations, and parallelisation

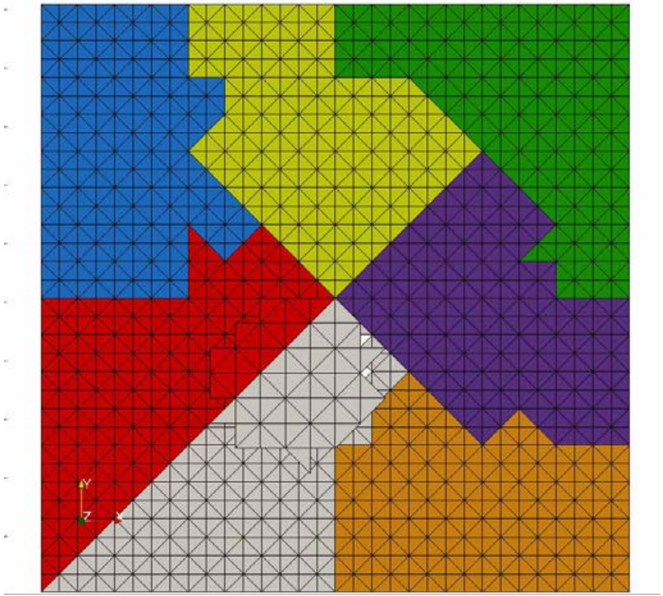


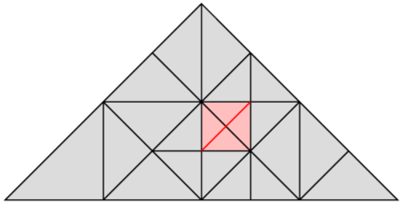


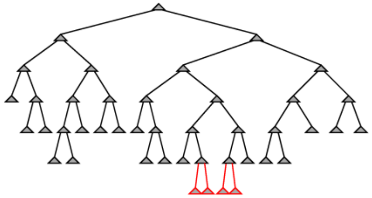
SFC #2 – Sierpinski: Tsunami Simulations

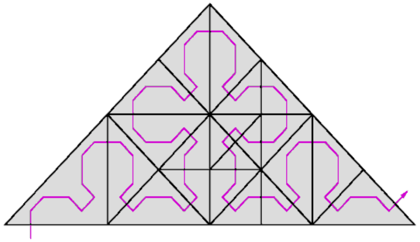
Sierpinski space-filling curves

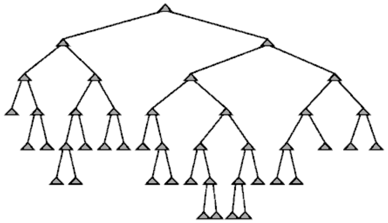
- FEM with strong adaptive refinement & coarsening
- structured, but triangular / tetrahedral
- high locality and HW-/cache-efficiency
- Sierpinski-based traversal, newest vertex bisection
- discontinuous Galerkin discretization
- **application: Tsunami simulation (shallow water eqs.)**

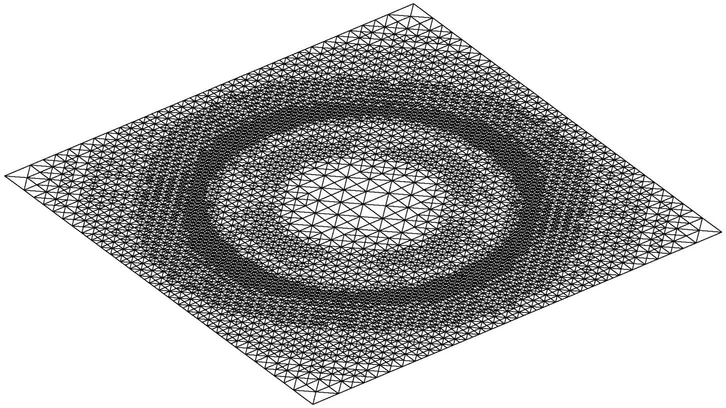












Part II – Peano: Space-Filling Curves for PDE Solvers

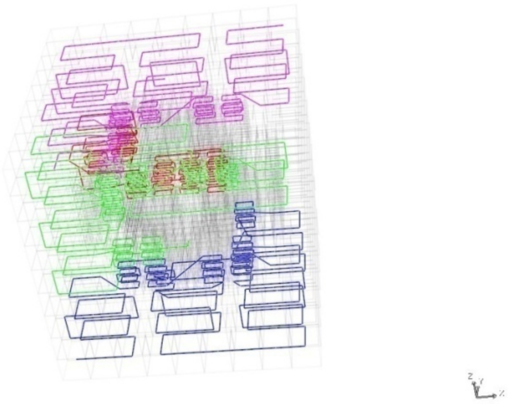
The Scope of Space-Filling Curves

The Peano Project

Applications

[not discussed here]

Yet Another Framework – *Ideas & Goals*



general PDE **framework**, with focus on CFD/FSI

discretization issue: FE – strictly conservative

grid issue: Cartesian – at least logically

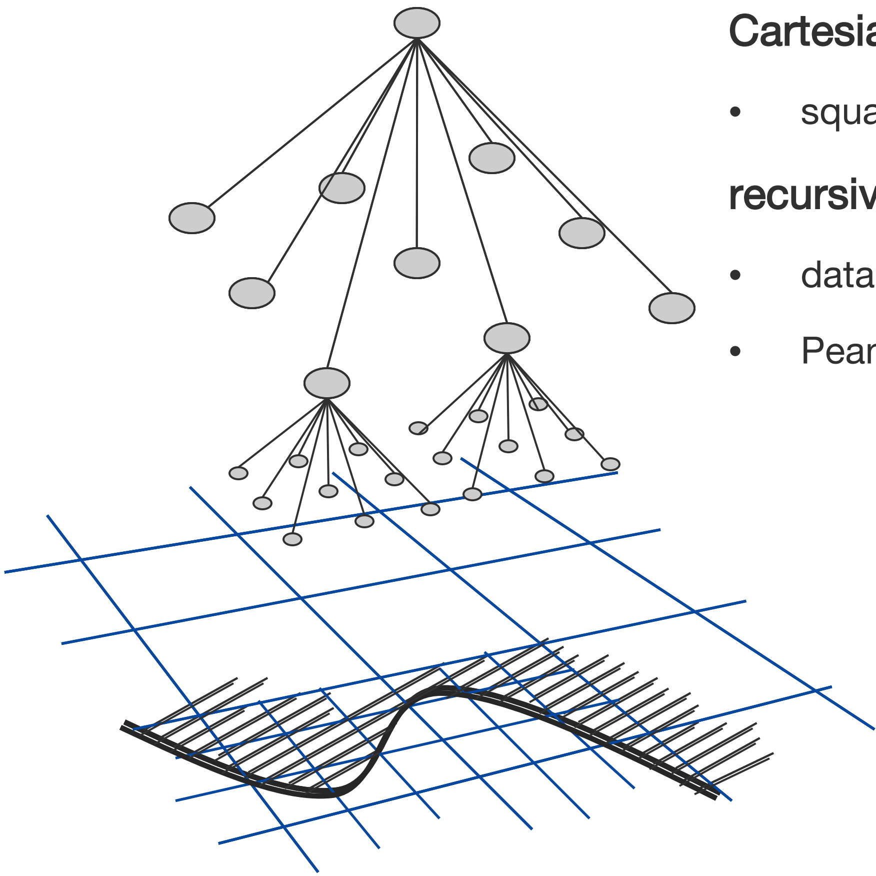
dynamics issue: straightforward generation & adaptation

solver issue: inherent multi-level solvers and parallelisation

dimensionality issue: general dimensionality

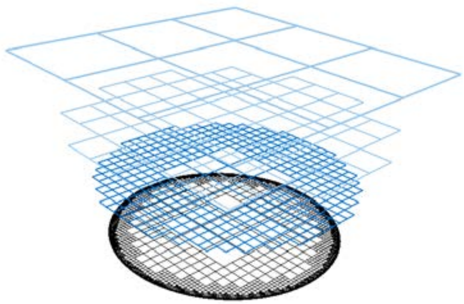
high **efficiency** (memory footprint w.r.t. size & access, parallel, ...)

Peano Concept #1: Grid Organisation via Spacetrees



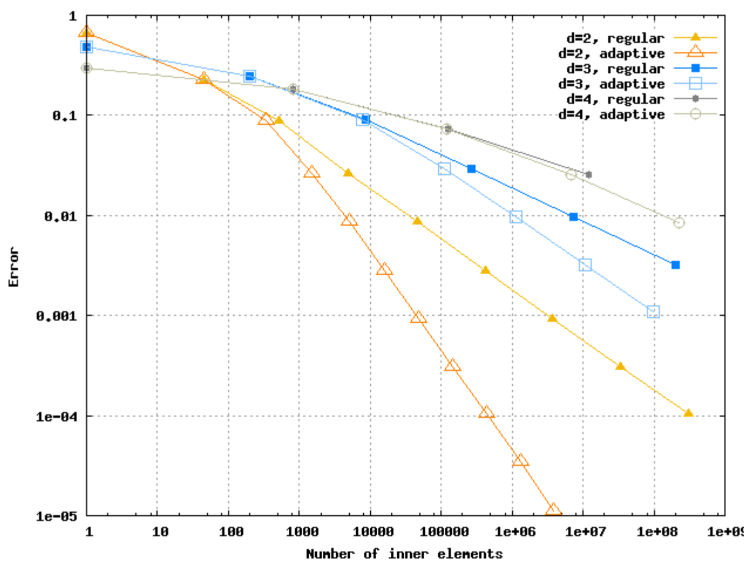
Cartesian grid cells

- squares/cubes/hypercubes

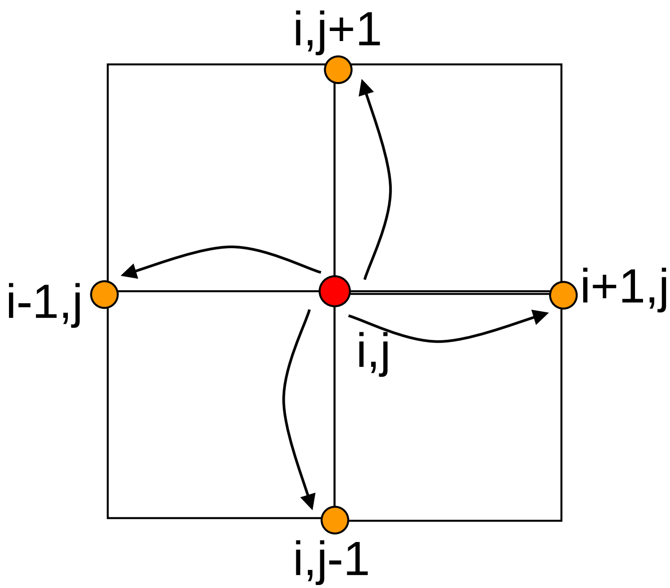


recursive refinement

- data structure: tree
- Peano: tri-partitioning



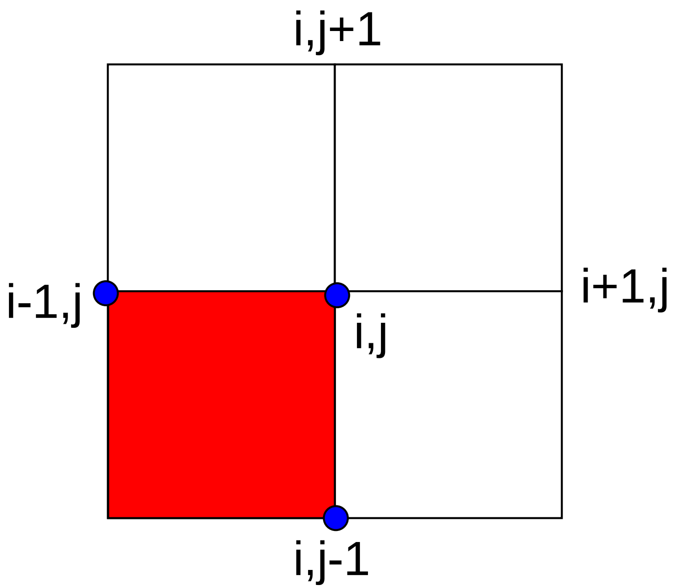
Peano Concept #2: Cell-Oriented Operator Evaluation



$$\begin{bmatrix} & 1 & \\ 1 & -4 & 1 \\ & 1 & \end{bmatrix}$$

$$(\Delta_h u_h)_{i,j} = \frac{u_{i-1,j} + u_{i,j-1} - 4u_{i,j} + u_{i+1,j} + u_{i,j+1}}{h^2}$$

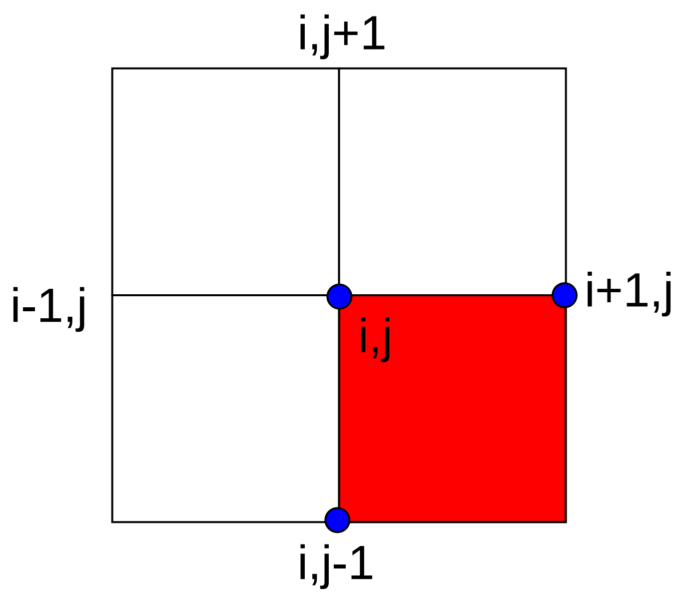
Peano Concept #2: Cell-Oriented Operator Evaluation



$$\begin{bmatrix} \frac{1}{2} & -1 & \\ & \frac{1}{2} & \end{bmatrix}$$

$$(\Delta_h u_h)_{i,j} = \frac{\frac{1}{2}u_{i-1,j} + \frac{1}{2}u_{i,j-1} - u_{i,j}}{h^2}$$

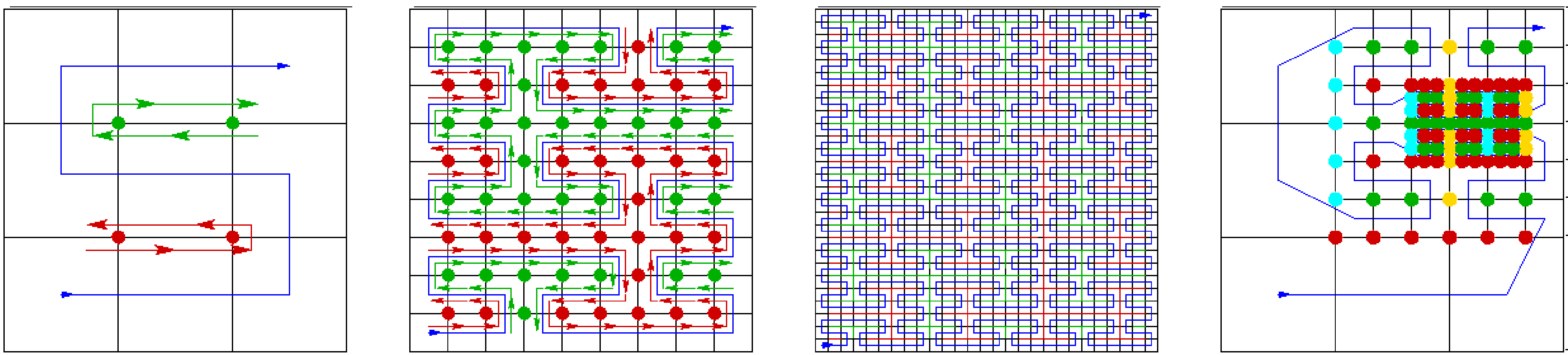
Concept #2: Cell-Oriented Operator Evaluation



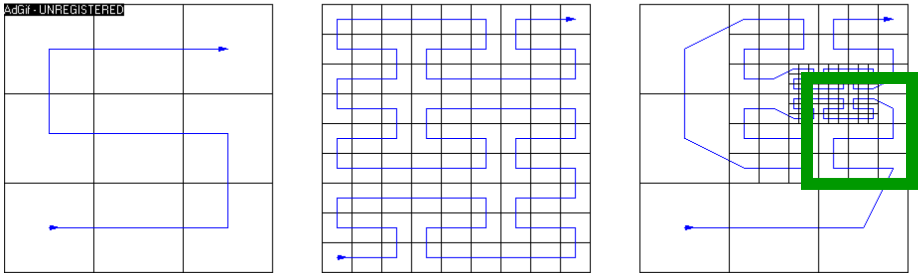
$$\begin{bmatrix} & & \\ & -1 & \frac{1}{2} \\ & \frac{1}{2} & \end{bmatrix}$$

$$(\Delta_h u_h)_{i,j} + = \frac{\frac{1}{2} u_{i+1,j} + \frac{1}{2} u_{i,j-1} - u_{i,j}}{h^2}$$

Peano Concept #3: Grid Traversal via Stacks



- traversal along a Peano curve ➔ also adaptive
- cell-oriented operator evaluation ➔ need for intermediate / non-persistent storage
- stacks as non-persistent data structure
- adaptivity & generating systems ➔ hierarchy
- high spatial and time locality of data access



Peano Features

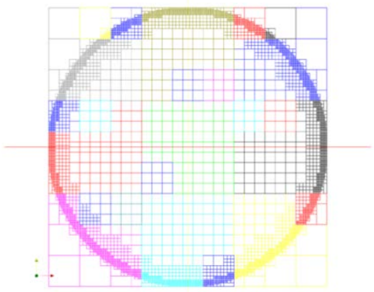
- dehierarchisation
- compute residual
- smooth
- restrict residual

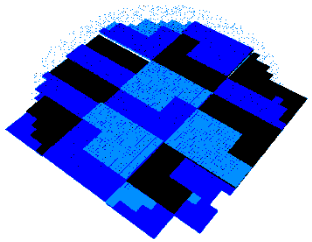
Feature #1: Multilevel inside

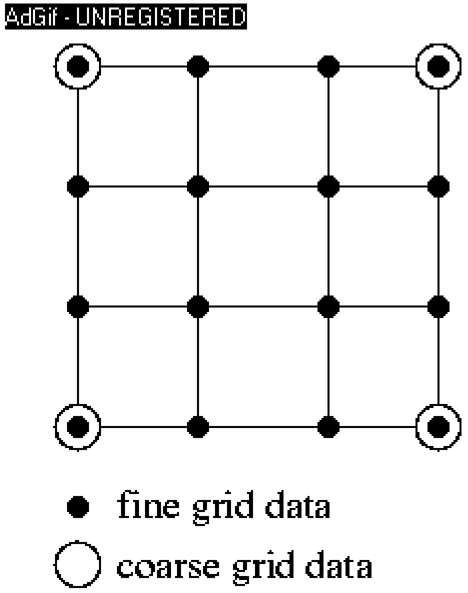
[exploits hierarchy – matrix-free concept, ML-preconditioned cg, multigrid, …]

Feature #2: Load balancing inside

[so far: works nice for moderate proc numbers up to O(10000)]



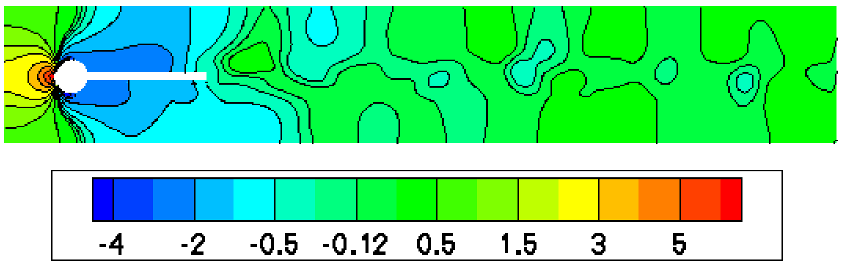


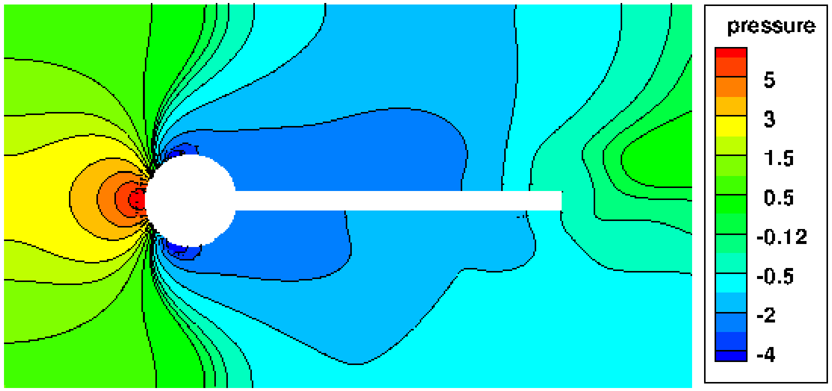


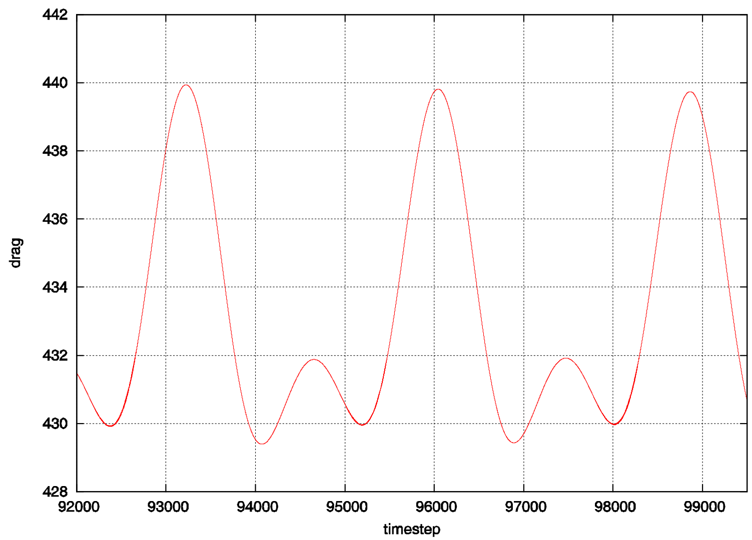
Feature #3: Efficient memory use and access

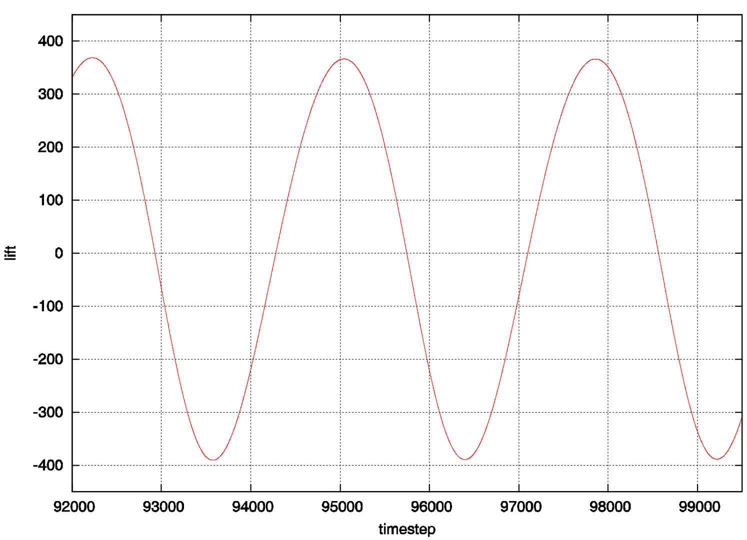
[throughout the hierarchy *disk* ←→ *main memory* ←→ *cache;* L2 hit rates > 99.9%]

FSI Fluid Solver Benchmark, Re = 200









Part III – Sparse Grids for High-Dimensional Numerics

Sparse Grids: Main Properties

First Applications: Quadrature and PDE (Flows, Finance)

[not discussed here]

Application to Classification & more

A Hot Topic: High-Dimensional Numerics

- **High:** not 2, not 3, not 3 plus time, but 10 … 100 ... 1000
- **Where?**
  - quantum mechanics
  - finance
  - parameter identification, optimisation (search in high-dim parameter spaces)
  - data mining, classification, information extraction
- **Why a problem?**
  - FEM: think of 11-dimensional hyper-tetrahedra and their adaptive refinement … ☺
  - Computational demand – the curse of dimension:
    - the simplest 1-D discretisation … … and in 100-D

$1^{100} = 1$

    - The second simplest 1-D discretisation … … and in 100-D

2^{100} approx. 10^{30}

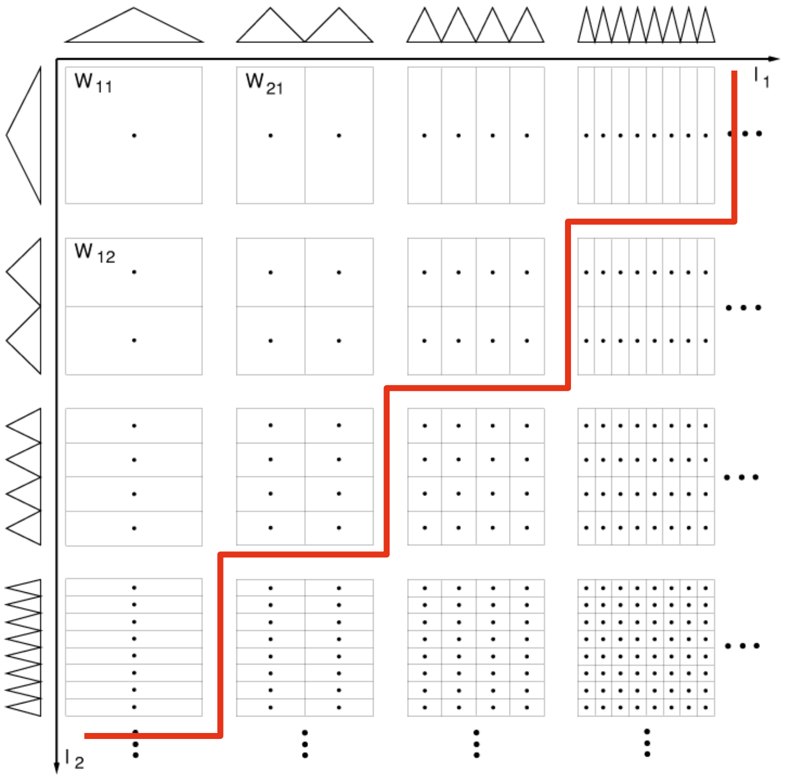
Sparse Grids in a Nutshell

- regularity: spaces *X(Ω)* of bounded mixed derivatives
- *d=1*: hierarchical bases (here linear)
- *d>1*: tensor product approach
- subspaces: basis functions with support of same aspect ratio
- discretization / approximation as an optimisation problem: find optimum choice of subspaces

$$\max_{u \in X(\Omega):\ |u|=1} \|u - u_{V(\mathrm{opt})}\|$$

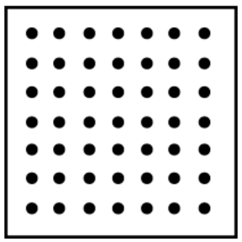
$$= \min_{U:\ |U|=N} \ \max_{u \in X(\Omega):\ |u|=1} \|u - u_U\|$$

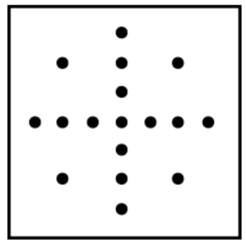
- result: sparse grids
  [Zenger et al., 1990]

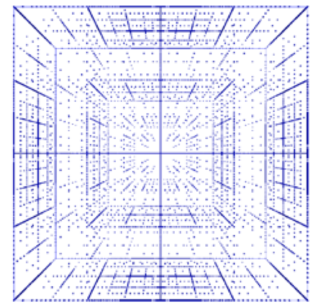


Sparse Grids in a Nutshell (cont'd)

- **Appearance:**

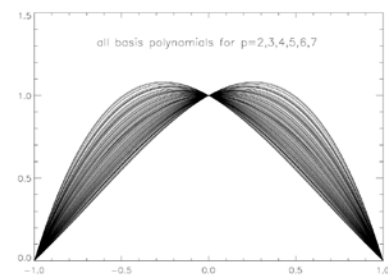






- **Cost** (number of grid points) vs. **benefit** (contribution to interpolant):
  (finest mesh width $h_n=2^{-n}$, hierarchical bases of piecewise degree p)

	sparse	full
# grid points	$O(h_n^{-1}\, n^{d-1})$	$O(h_n^{-d})$
error (max, L_2)	$O(h_n^{p+1}\, n^{d-1})$	$O(h_n^{p+1})$
error (energy)	$O(h_n^{p})$	$O(h_n^{p})$



- Extensions: straightforward access to **adaptive refinement**, generalisation to **piecewise polynomial** hierarchical bases, energy-optimal sparse grids

Part III – Sparse Grids for High-Dimensional Numerics

Sparse Grids: Main Properties

First Applications: Quadrature and PDE (Flows, Finance)
[not discussed here]

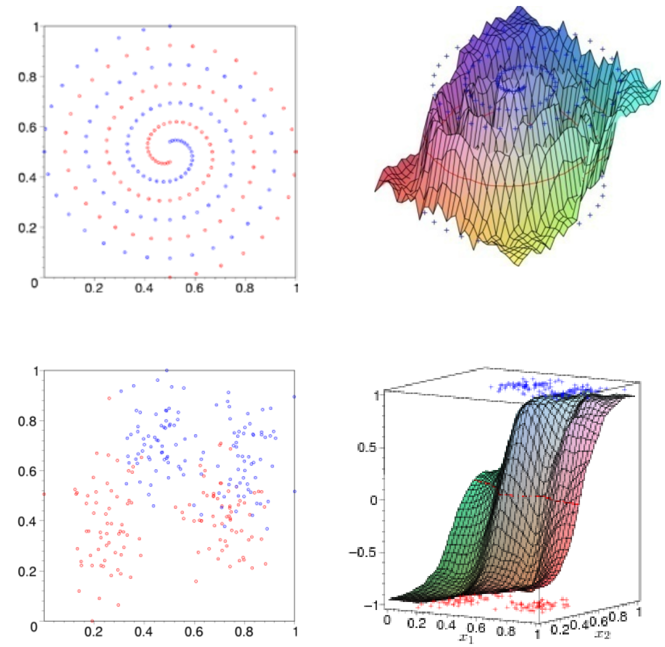
Application to Classification & more

Classification & Regression in Data Mining

- **Problem:** machine learning of a 2-class problem
- Given a **pre-classified data set**

$$S = \{(\mathbf{x}_i, y_i) \in [0,1]^d \times \{-1,1\}\}_{i=1}^{M}$$

of normalized data points $\mathbf{x}_i$ with class labels y_i
(regression: real numbers instead of discrete labels)



- **Typically: presence of noise**
  [sampling ➔ noise ➔ no mere interpolation]

- **Computational task:**
  – construct classifier/ machine learner (ML)

$$f : [0,1]^d \to \{-1,1\}$$

  – provides class predictions applied to new data points

Regularization Network Approach

- Classification as **scattered data approximation problem** *plus* additional regularization terms (ill-posed problem, noise):

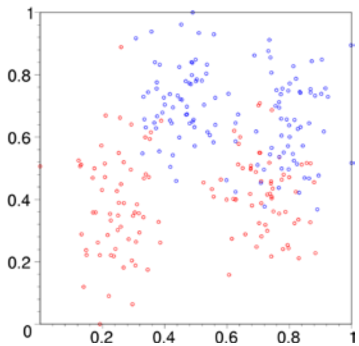
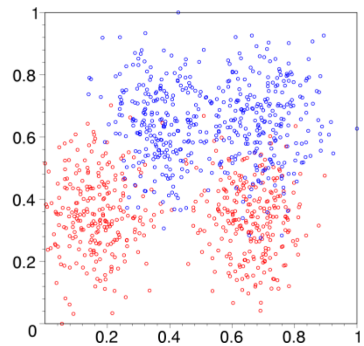
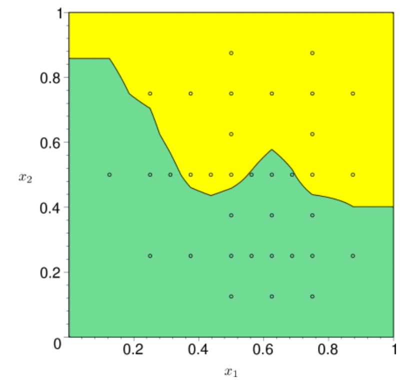
$$\text{minimize } H[f] = \frac{1}{M}\sum_{i=1}^{M} \mathcal{V}(y_i, f(\mathbf{x}_i)) + \lambda \|f\|_K^2$$

  - cost/error function, for example $\mathcal{V} := (y_i - f(\mathbf{x}_i))^2$
  - regularization operator/stabilizer, for example $\|f\|_K^2 := \|\nabla f\|_{L_2}^2$
  - simpler, but astonishingly useful $\text{minimize } H[f] = \frac{1}{M}\sum_{i=1}^{M}(y_i - f(\mathbf{x}_i))^2 + \lambda \sum_{i=1}^{N} \alpha_i^2$
  - regularization parameter λ , $f_N(\mathbf{x}) = \sum_{i=1}^{N} \alpha_i \phi_i(\mathbf{x})$
- Minimize trade-off between cost and smoothness via λ
- Various approaches (neural networks, support-vector-machines) can be formulated as Regularization Network Approach
- Common classification algorithms:
  - discretization of feature space not feasible (curse of dimension, $O(N^d)$)
  - global ansatz functions associated to data points ($O(M^2)$, large training data?)
- Idea: use sparse grids, i.e. a *data-set-independent* approach

Examples

Ripley data set (*d=2*)

- training (250) and test data (1000), 8% noise (i.e. 92% maximum accuracy)
- most refinement in critical region, accuracy of 91.5% on test data
- after only 8 refinement steps, overfitting takes over and accuracy deteriorates

Bupa liver data set (345 patients for liver illness, *d=6*, λ*=0.01*)

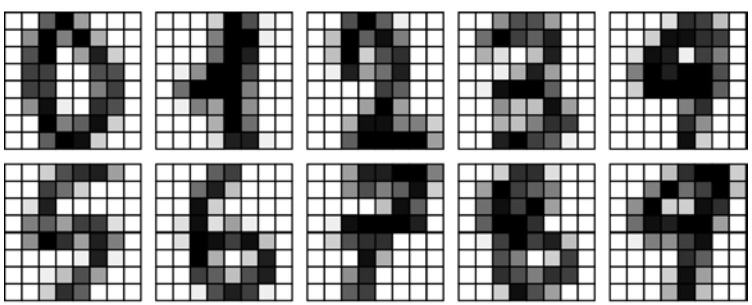
adapt. sg $\lambda = 0.01$ # refinements	|grid|	acc. [%]	comb. techn. lin. anisotrop. acc. [%]	SVM linear acc. [%]	SVM non-linear acc. [%]
7	403	72.22	73.9	70.0	73.7
13	1091	74.61			
15	1371	76.30			

Towards Higher Dimensionalities

Optical recognition of hand-written digits, *d=64*

- 8x8 pattern of grey-scale values, 3,823 training and 1,797 test data
- one classifier for each class (ten successive 2-class problems)
- result: **97.74%**

  compared to k-NN: 98.00%
  compared to RBF-DDA networks: 97.45%
  compared to Tree-SVM: 97.27%
  compared to MLP: 89.05%
- grid points on each level for one of the classifiers (no boundary points)
- adaptive refinement crucial

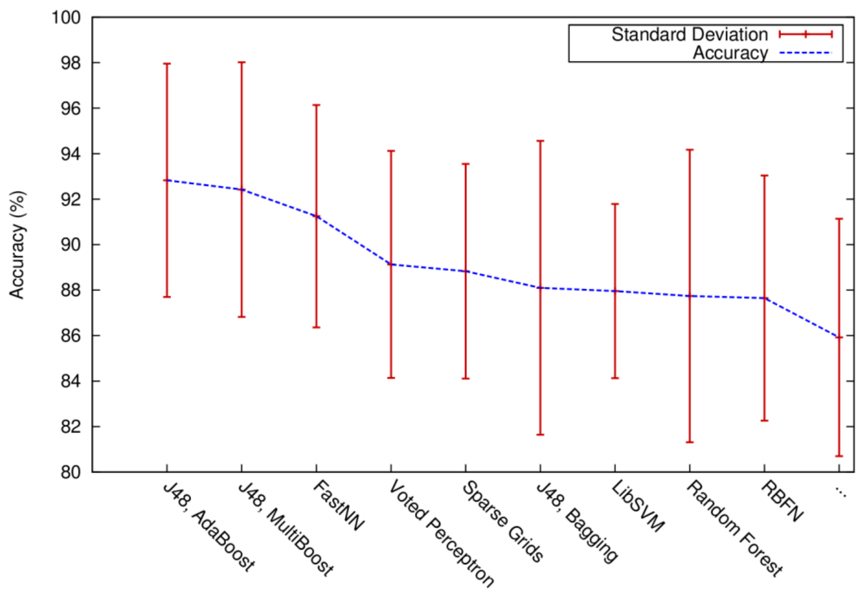


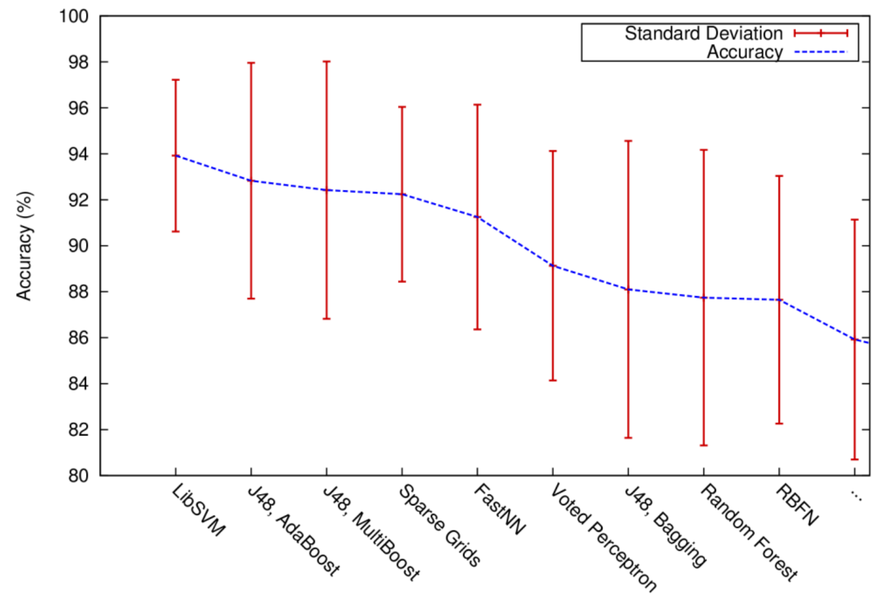
Level	Regular Sparse Grid	Adaptive Sparse Grid
1	1	1
2	128	128
3	8,324	993
4	366,080	510
5	12,263,680	128

Towards Higher Dimensionalities

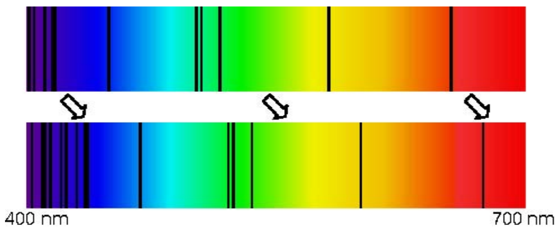
Musk data sets, *d=166*

- separate molecules (166 attributes, mainly describing distance features of conformations)
- 10x 10-fold cross-validation
- M=476 (left) and smaller data set (right, with PCA leading to *d=35*)
- only two refinements before PCA, more possible after PCA
- benchmark study done 2008 to compare 45 classification algorithms; best 9 out of 38



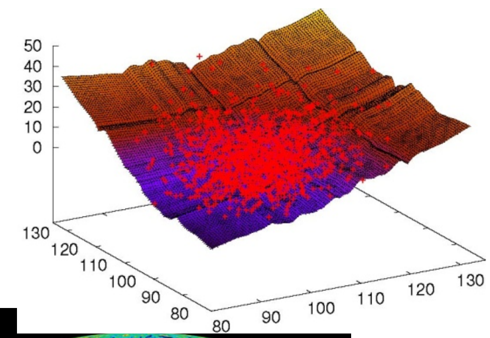


Applications of Regression

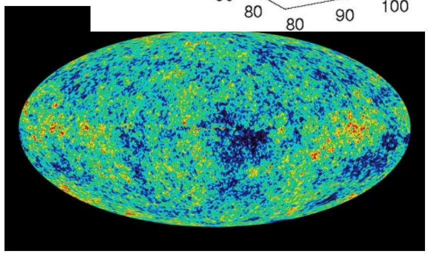


- **Cosmological redshift estimation**

  [use cheap photometric measurements to predict expensive, but accurate spectroscopic ones; 5D; large data set: 430 k data points, 60 k used for testing]

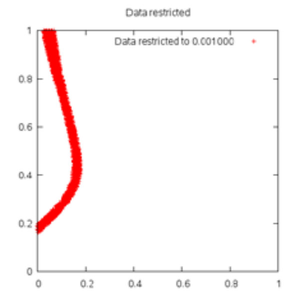


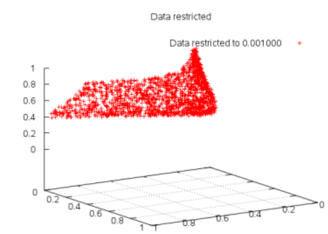
- **Option pricing**



- **Cosmological parameter sampling**

  [cosmic microwave background radiation emitted just after Big Bang; 6-9 parameters; model available; compare results with observations; determine the best/most probable set of parameters (inverse problem); so far stochastic approaches only]



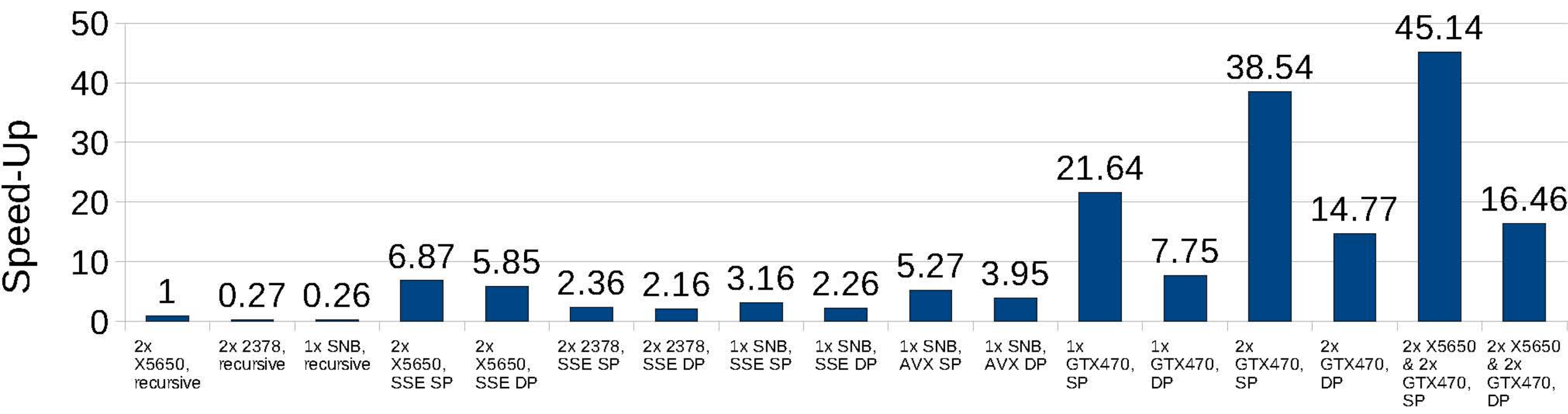


- **Parameter scans in plasma physics**

  [task arising in gyrokinetics, quasi-linear model; part of optimization problem; aim: interpolate]

Lessons Learned

- Efficient parallelization possible



Part I – General Remarks

Part II – Peano: Space-Filling Curves for PDE Solvers

Multi-physics
Multi-scale
Multi-level

Part III – Sparse Grids for High-Dimensional Numerics

Multi-dimensional

Thanks to all those who really did the work

&

Thanks for your attention!