FEAST: The Future

(Finite Element Analysis & Solution Tools)

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Germany

Overview

- Performance
- Solver
- FEAST structure

Performance

Where to calculate the world?

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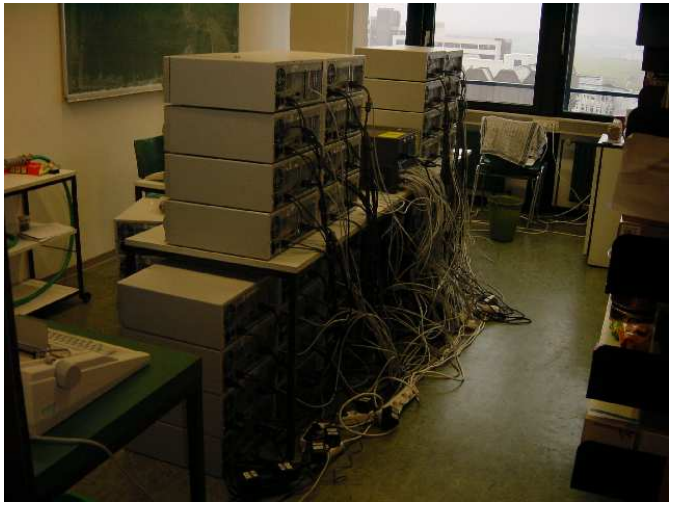

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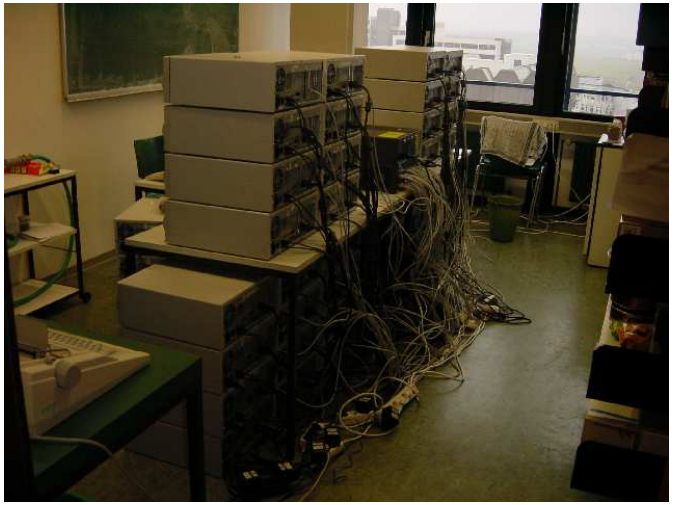

vector system:

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- utilisation of vector capabilities and built in CPU features
- automatic parallelization but only efficient for #CPU < 8
- but no other way with respect to memory and CPU requirements for realistic numerical simulation

How to measure 'Performance'

Linpack test, Gaussian Elimination, benchmark for the TOP500 list

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Rank	Name	Rmax $GFlop/s$	Site	#CPU
1	IBM ASCI White,SP Power3 375 MHz	7226	LLNL USA	8192
2	Compaq AlphaServer SC ES45/1 GHz	4059	Pittsburgh SC USA	3024
3	IBM SP Power3 375 MHz	3052	NERSC/LBNL USA	3328
10	IBM SP Power3 375 MHz	1293	DWD Germany	1280
17	Hitachi SR8000-F1/112	1035	Leibniz RZ Germany	112
21	Fujitsu VPP5000/100	886	ECMWF UK	100
30	Self-made CPlant/Ross Cluster	706	Sandia USA	1369
500	Cray Inc. T3E1200	94	EPA USA	116

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But typical situation in high performance computing today:

Example: STAR-CD ($k-\epsilon$), 500 000 cells (by Daimer Chrysler), SGI Origin2000 (6 CPUs), 6.5 CPU h

Quantity	Experiment	Simulation	Difference
Drag ('c_w')	0.165	0.317	**92 %**
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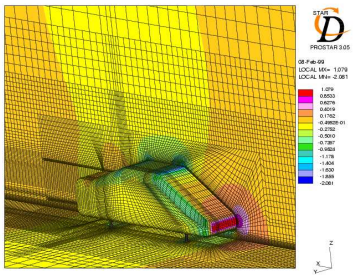

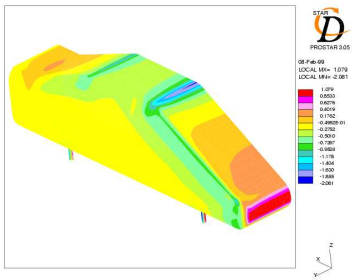

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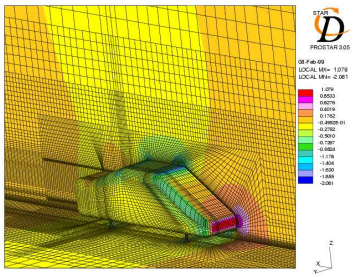

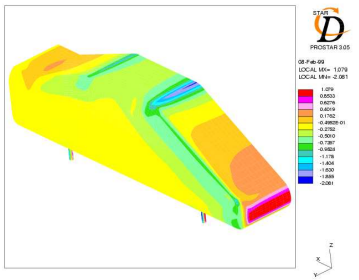

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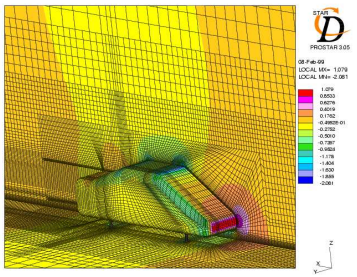

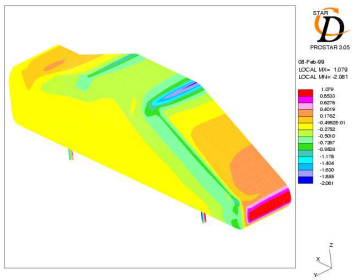

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- Are special strategies necessary to exploit the performance?

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AMD Athlon XP 1500+ with 1333Mhz core frequency, measured MFlop/s

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N	case 1	case 2	case 3
500	323	477	940
1000	275	481	1119
3000	116	152	1362

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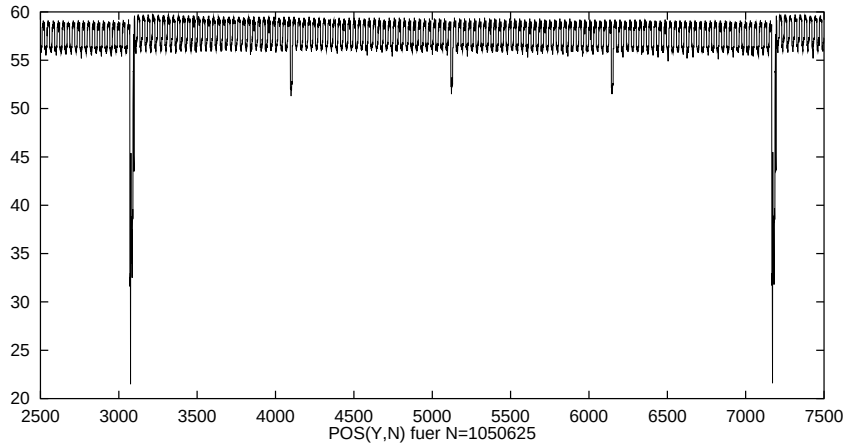

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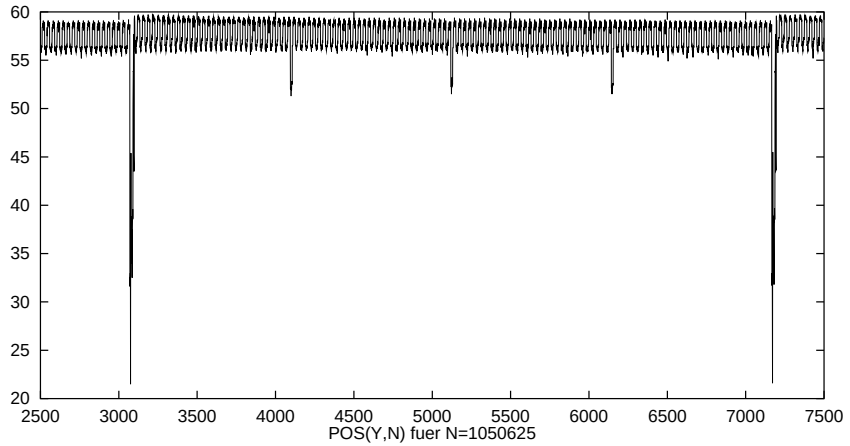

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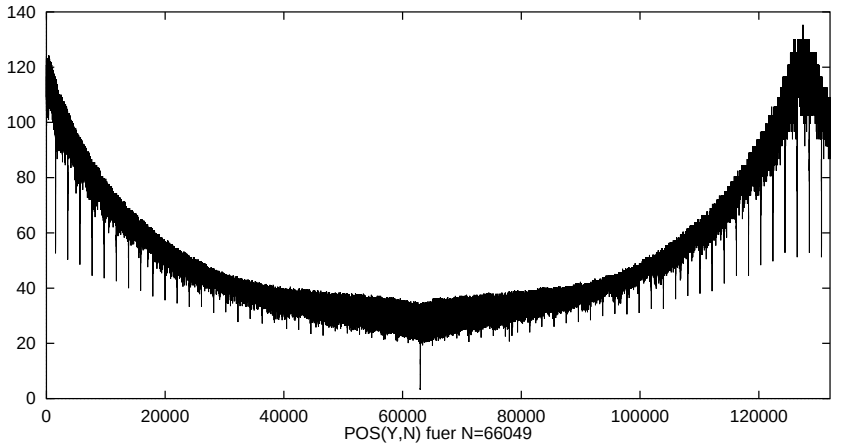

Sun U450

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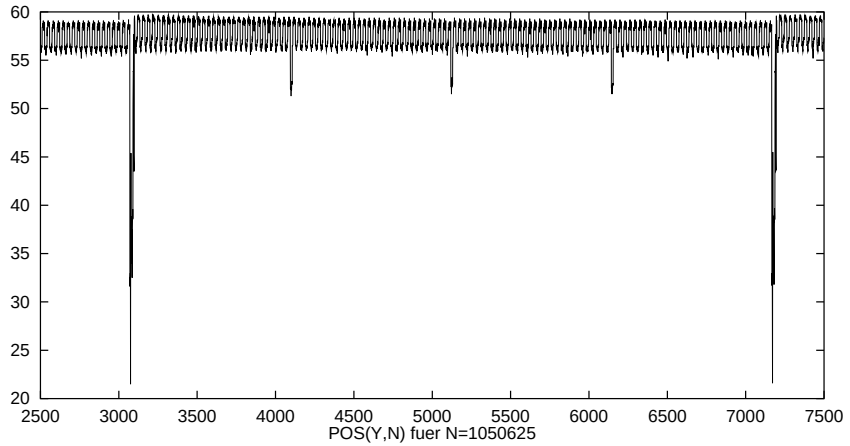

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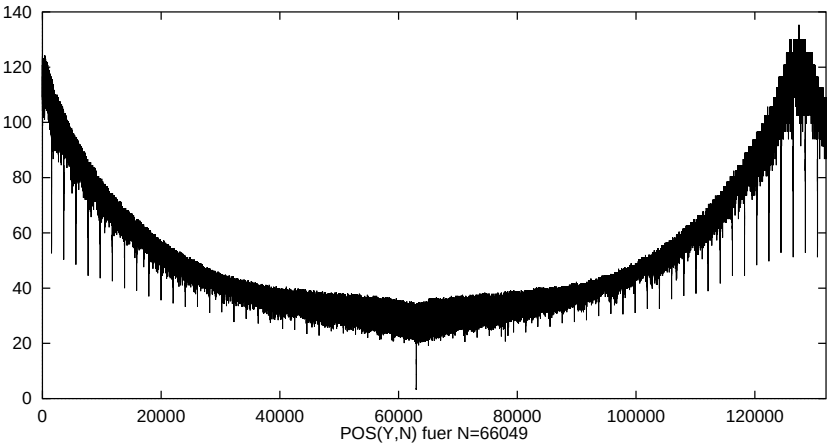

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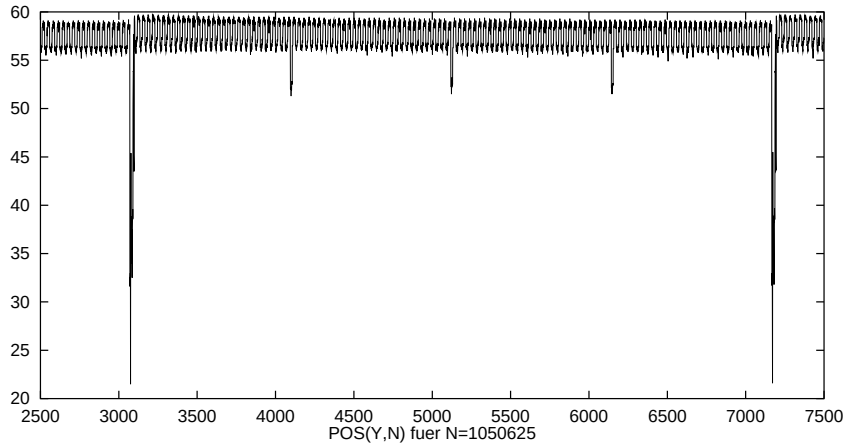

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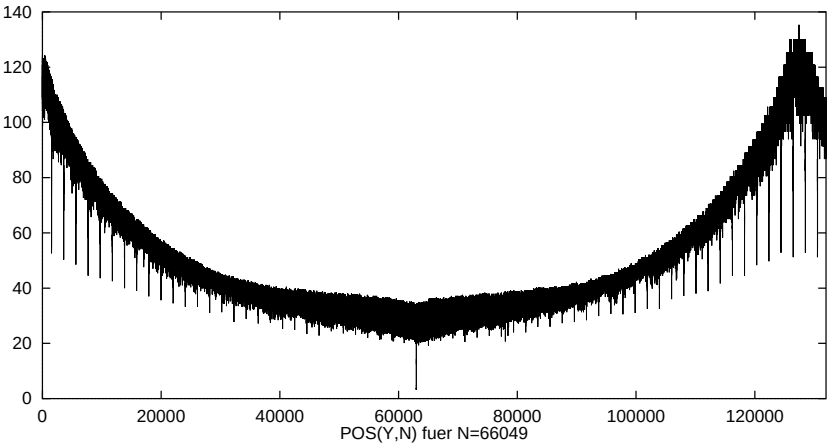

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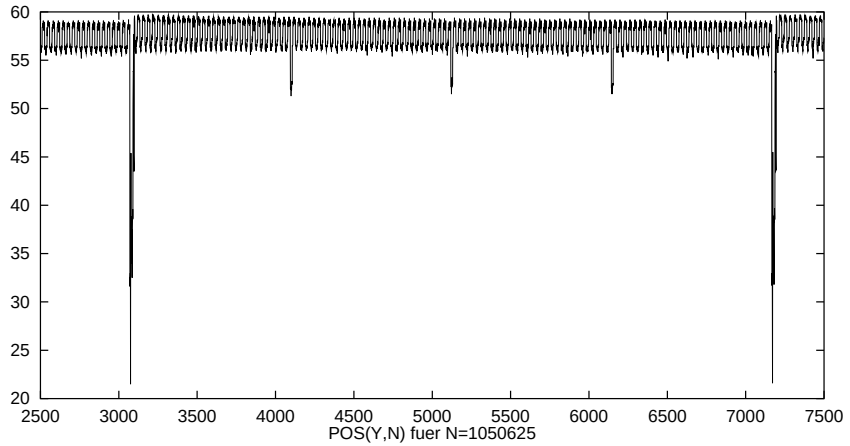

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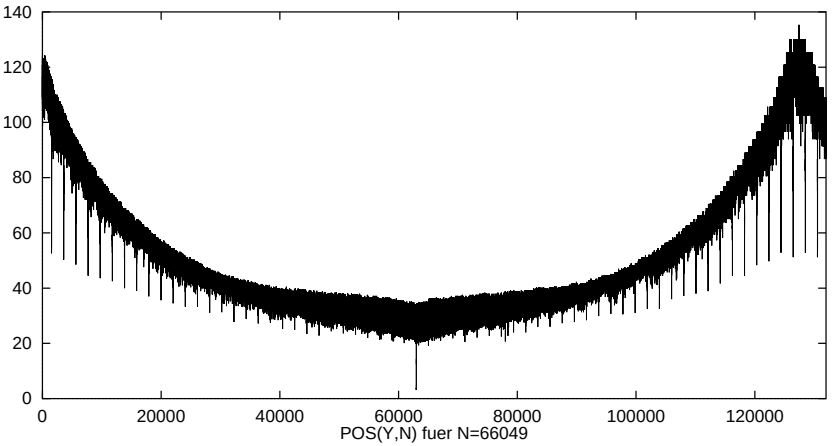

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- small ’windows’ of higher performance
- how to control the memory position ???

Sparse Matrix Vector Multiplication

Standard sparse matrix vector algorithm:

(DAXPY indexed)

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DO 10 IROW=1,N
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- different numberings can lead to identical numerical results and work (w.r.t. arith.ops and data accesses) but to huge differences in CPU time
- sparse techniques 'slow' and depend on problem size and kind of data access

Alt.: Sparse Banded Techniques

Question: How to exploit more performance?

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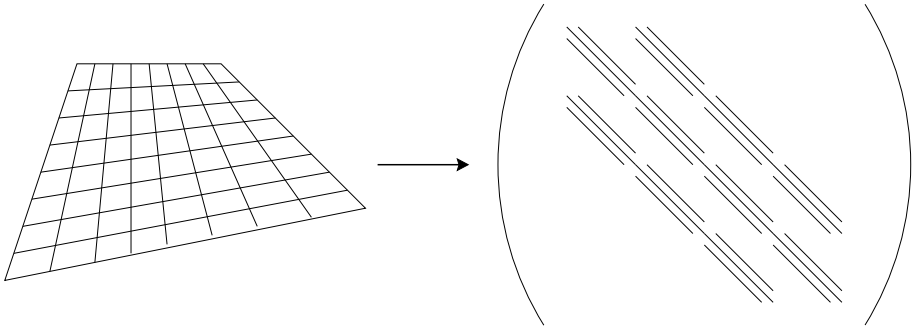
Line- or rowwise numbering:



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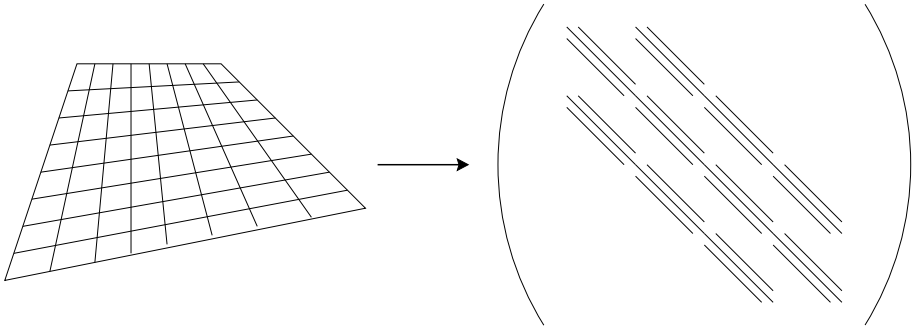

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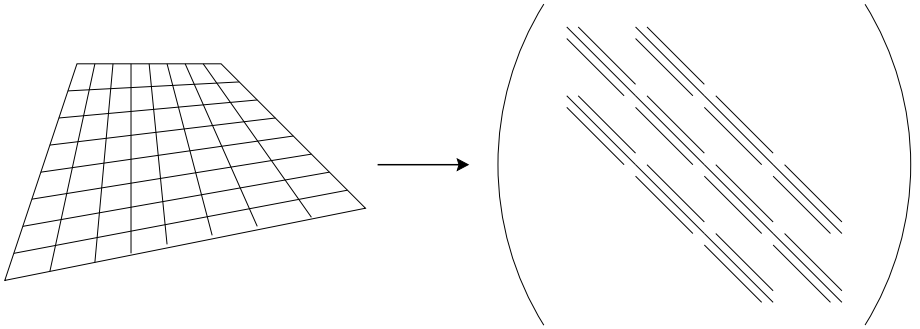

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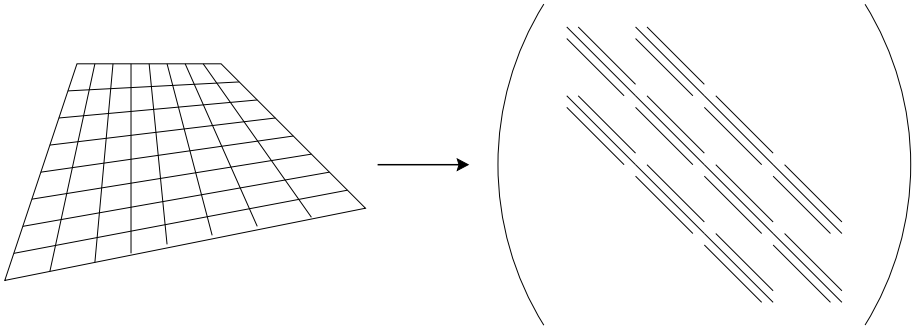

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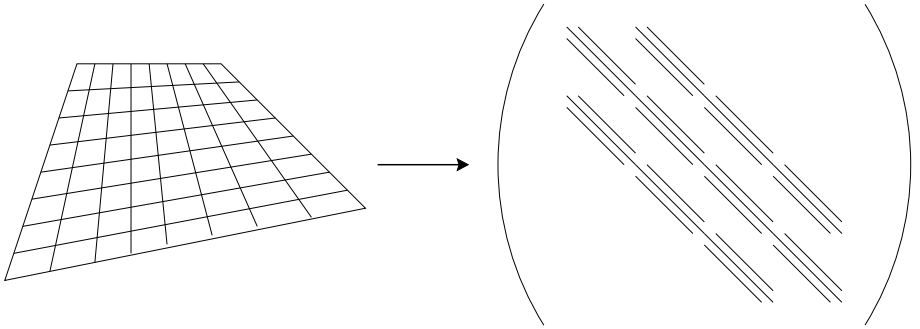

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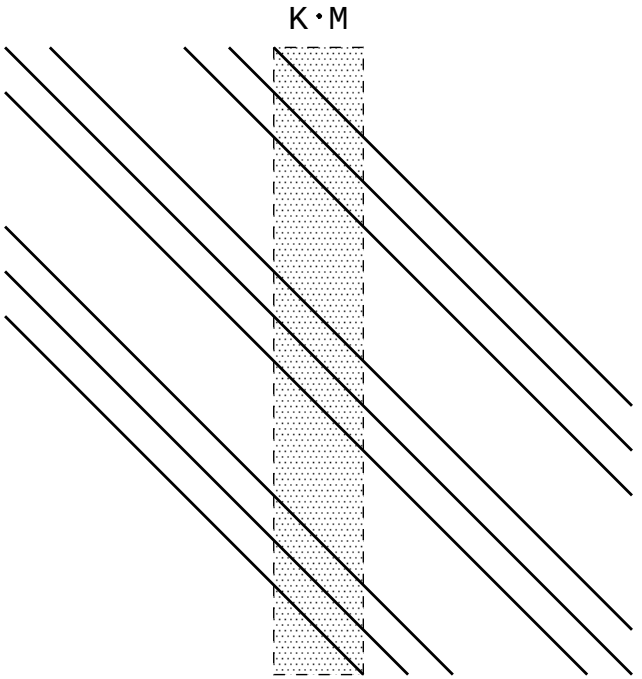
- matrix vector multiplication 'bandwise'
- in equidistant case for certain operators diagonals are constant

Sparse Banded Techniques I

Bandwise windowed multiplication (variable, constant):




```
DO 1 IM=1,M/K
  DO 2 I=1,K*M
2 Y(I) =Y(I) +DD(I)*X(I)+DL(I)*X(I-1)+DU(I)*X(I+1)
  DO 3 I =1,K*M
3 Y(I-M)=Y(I-M)+LD(I)*X(I)+LL(I)*X(I-1)+LU(I)*X(I+1)
  DO 4 I=1,K*M
4 Y(I+M)=Y(I+M)+UD(I)*X(I)+UL(I)*X(I-1)+UU(I)*X(I+1)
1 CONTINUE
```

Sparse Banded Techniques II

2D case	N	DAXPY-I	SBB-V	SBB-C	**MG-V**	**MG-C**
DEC 21264	65^2	205 (178)	538	795	370	452
(667 MHz)	257^2	224 (110)	358	1010	314	487
'**ES40**'	1025^2	**78 (11)**	**158**	**813**	**185**	**401**
HITACHI	65^2	173 (82)	238	391	191	266
(375 MHz)	257^2	143 (29)	243	388	198	260
'**SR8000**'	1025^2	**144 (7)**	**226**	**390**	**200**	**267**
AMD K7	65^2	203 (195)	101	556	122	355
(850 MHz)	257^2	29 (27)	78	241	72	166
'**ATHLON**'	1025^2	**31 (10)**	**64**	**236**	**58**	**126**

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'**ES40**'	1025^2	**78 (11)**	**158**	**813**	**185**	**401**
HITACHI	65^2	173 (82)	238	391	191	266
(375 MHz)	257^2	143 (29)	243	388	198	260
'**SR8000**'	1025^2	**144 (7)**	**226**	**390**	**200**	**267**
AMD K7	65^2	203 (195)	101	556	122	355
(850 MHz)	257^2	29 (27)	78	241	72	166
'**ATHLON**'	1025^2	**31 (10)**	**64**	**236**	**58**	**126**

Question: How to use these techniques on complex domains?

Sparse Banded Techniques II

2D case	N	DAXPY-I	SBB-V	SBB-C	**MG-V**	**MG-C**
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Question: How to use these techniques on complex domains?

$\Rightarrow$ **ScaRC**

FEAST Indices I

Framework of different numerical linear algebra tests for different problem sizes, using the Sparse Banded BLAS routines

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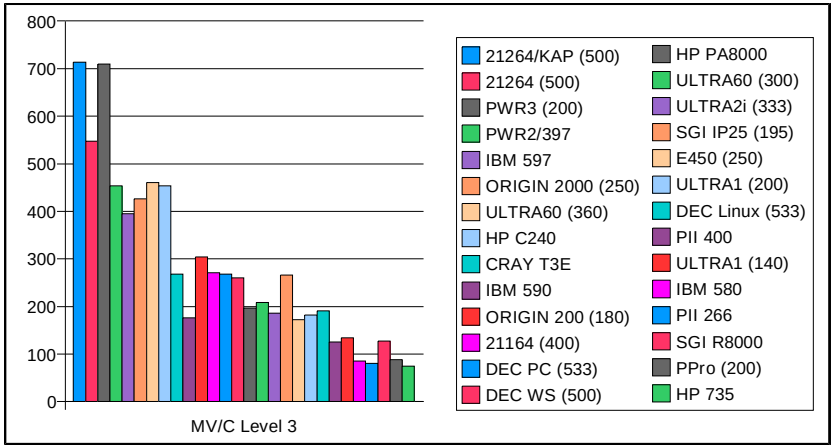

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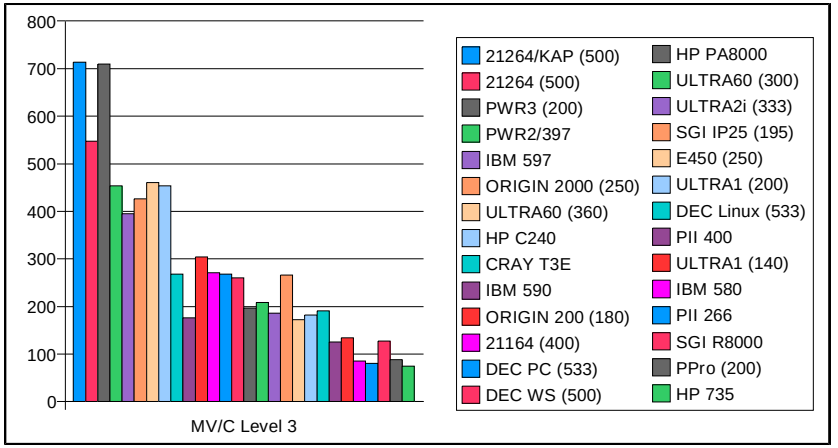

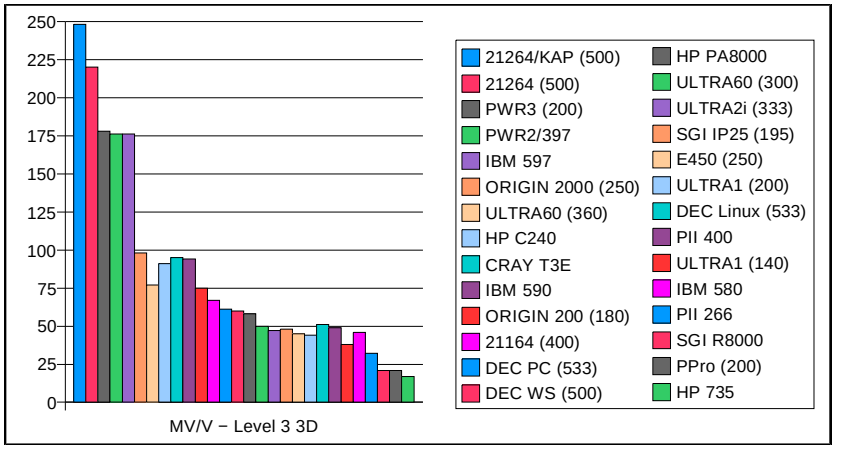

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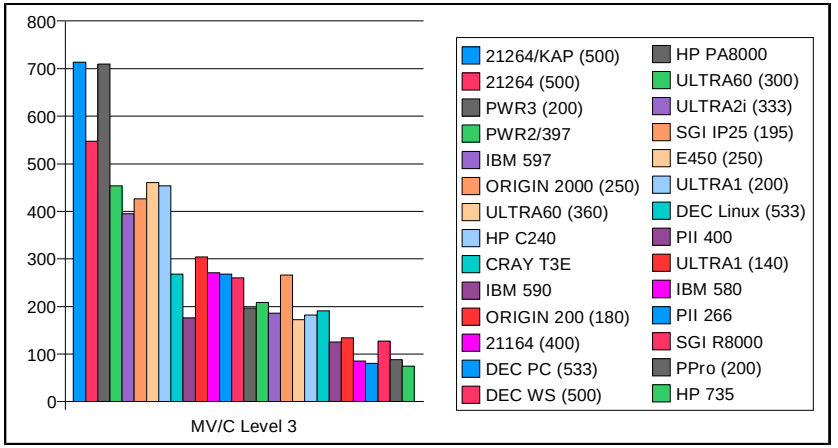
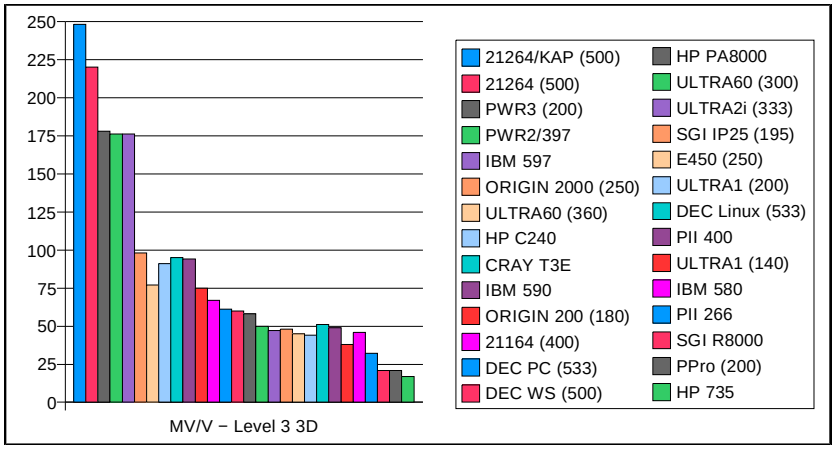
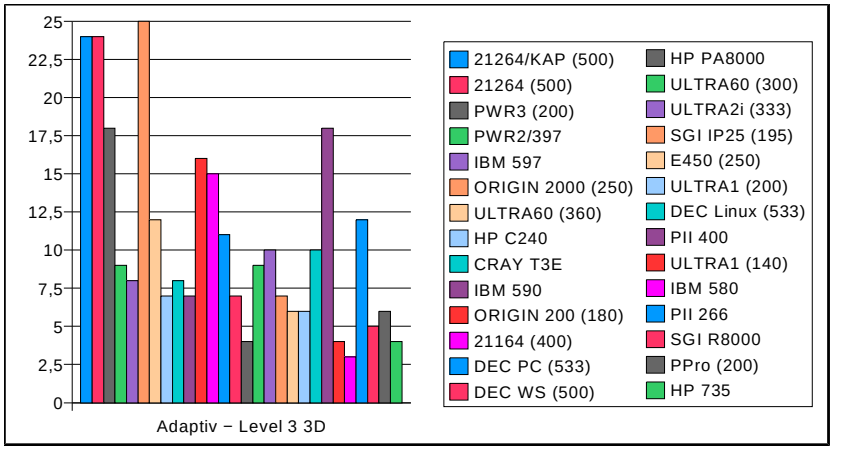
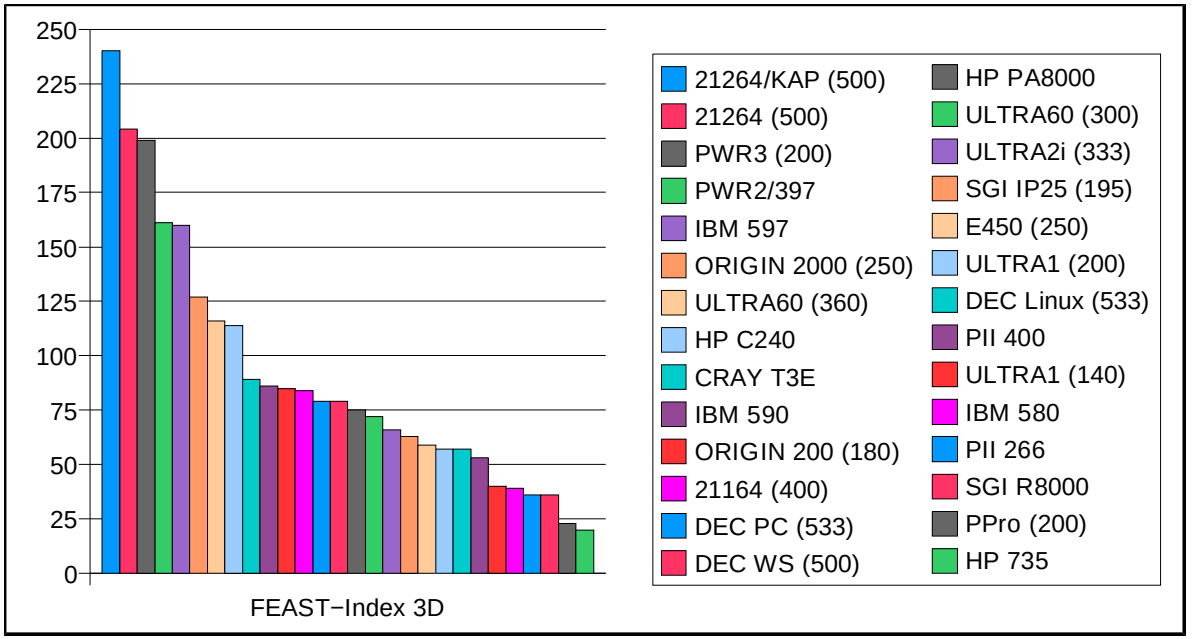






FEAST Indices II

Observations:



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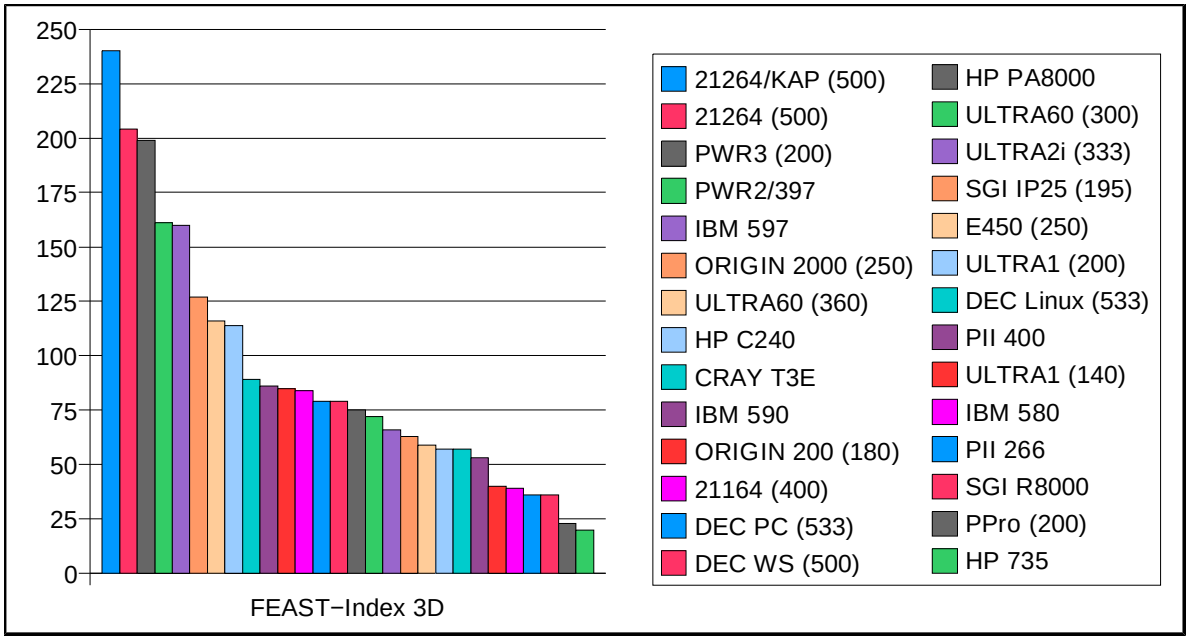

Observations:

- MFLOP rate for standard sparse techniques far away from peak performance, depending on problem size and numbering of the unknowns

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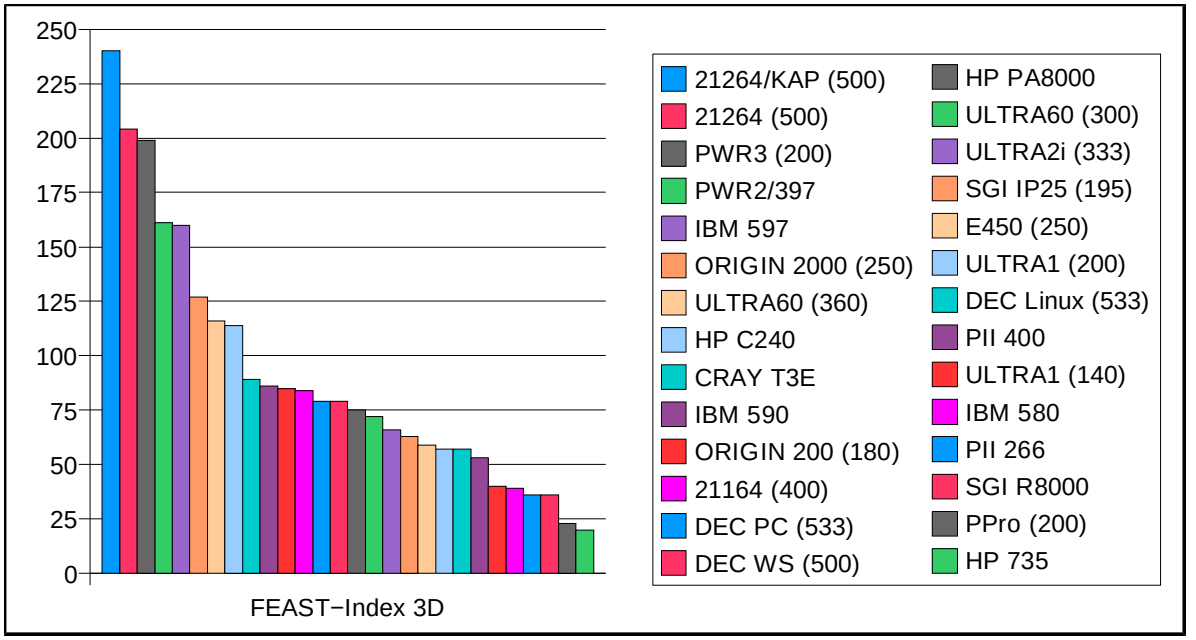

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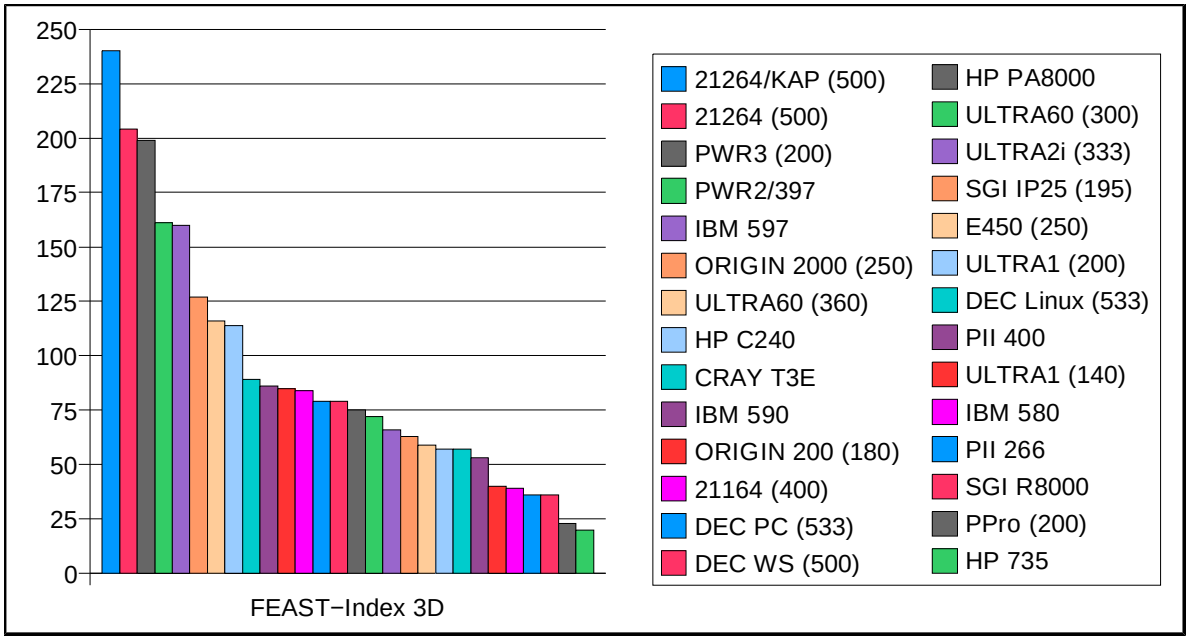

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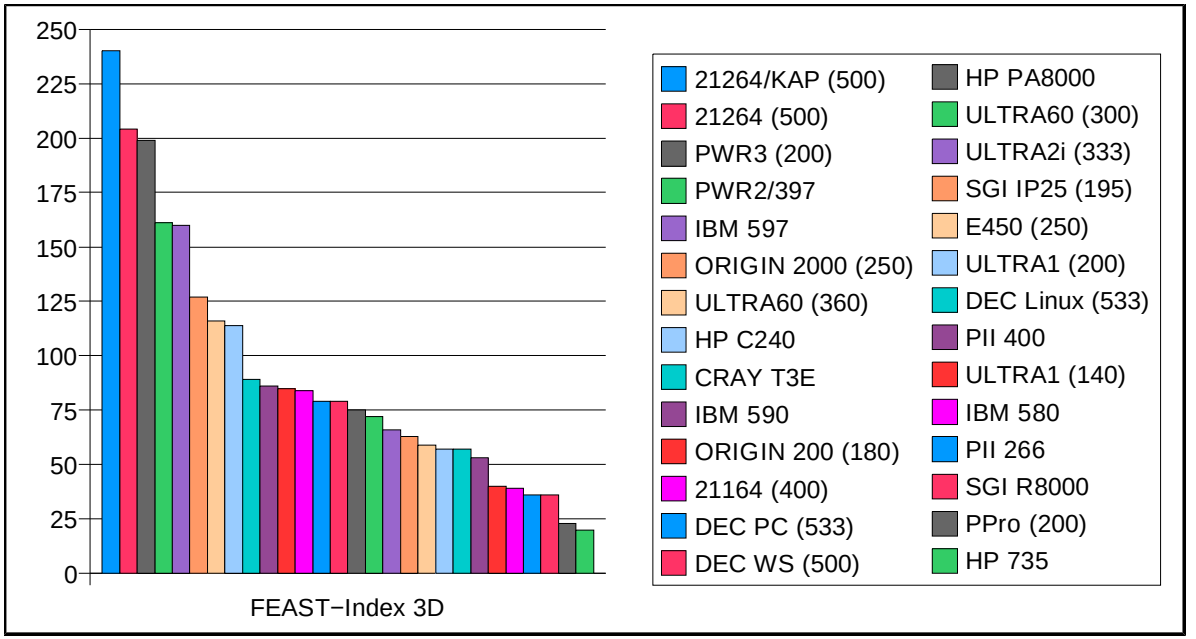

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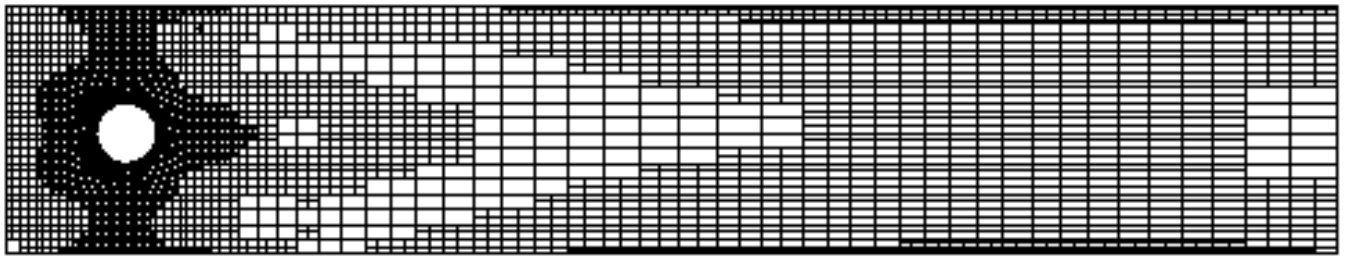
Solver

Hierarchical Divide and Conquer

Optimal grid for drag–coefficent via a posteriori error estimation:



(ROLAND BECKER, INST.F.ANG.MATH., UNIVERSITÄT HEIDELBERG)

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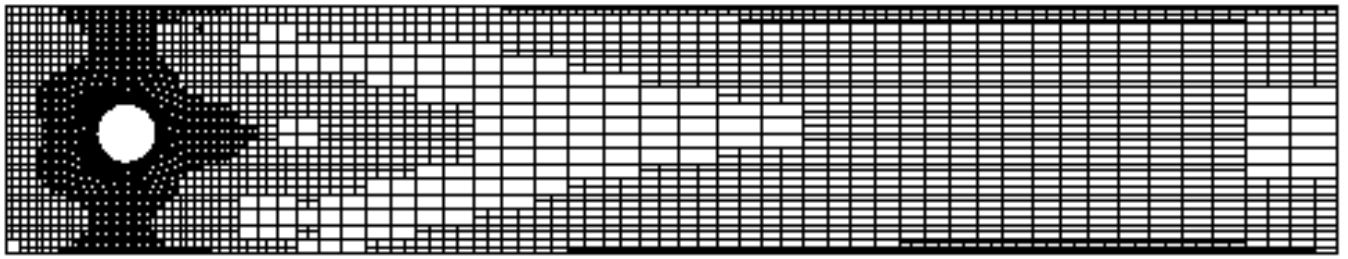

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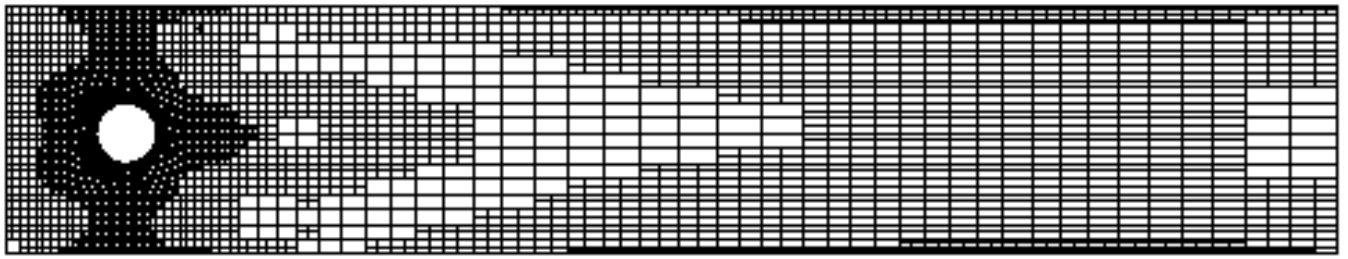

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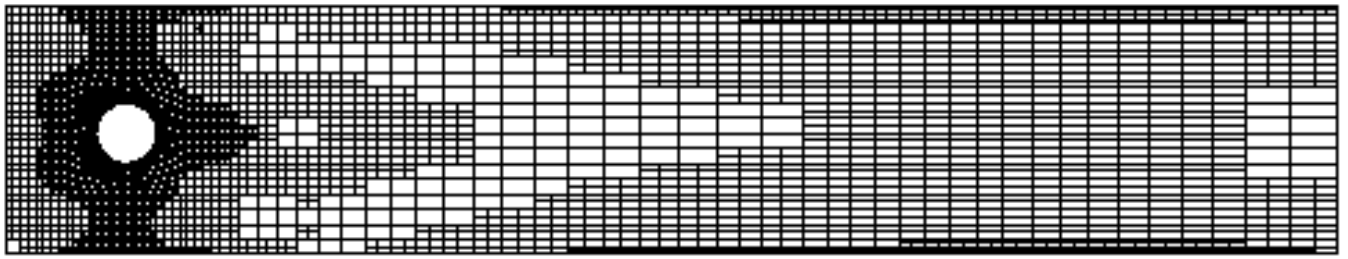

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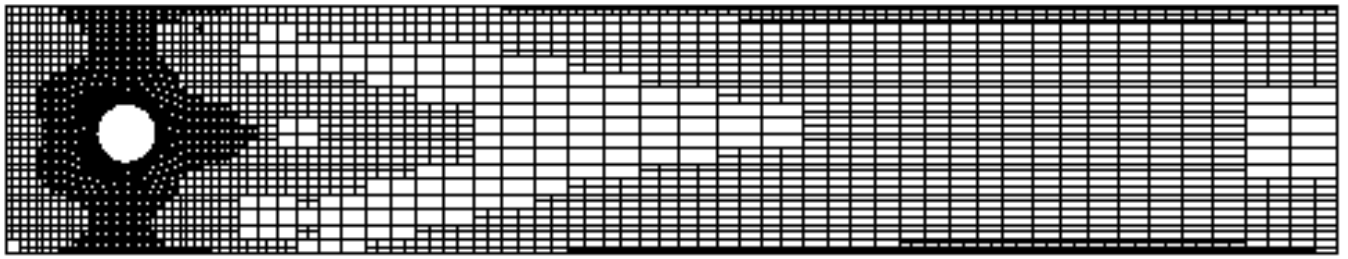

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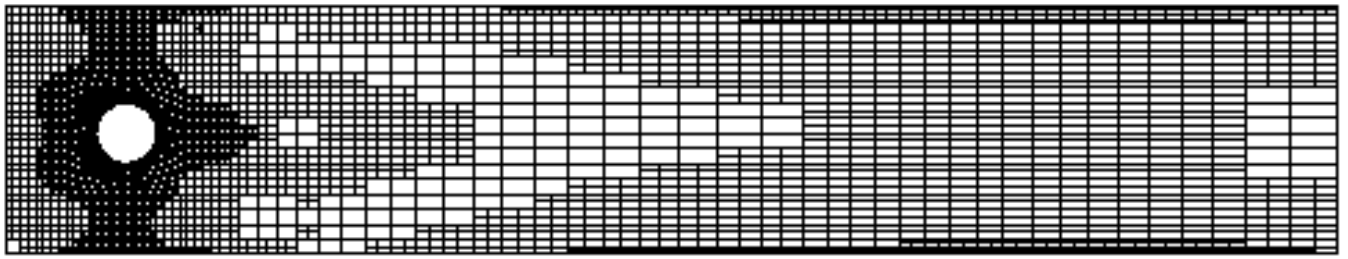

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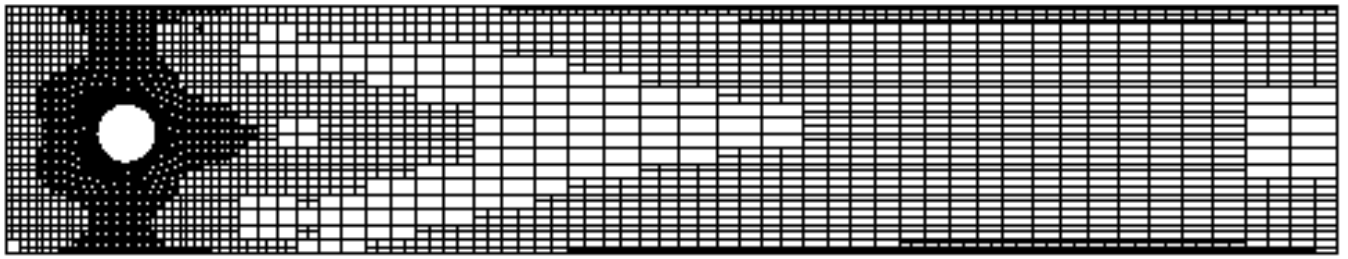

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- adaptive techniques only locally near boundaries
- regular substructures (90 %) in interior
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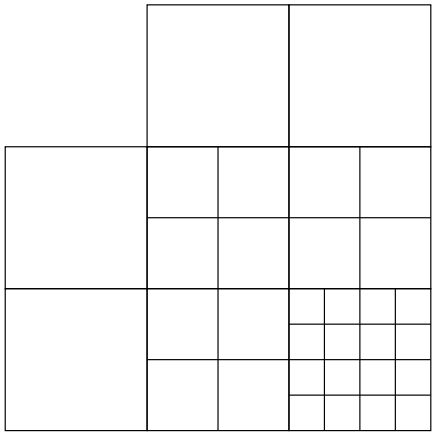
- recursive **Divide and Conquer** strategy
- find locally structured parts (high performance)
- find locally anisotropic parts (hide locally, robustness)

Hierachical Structures



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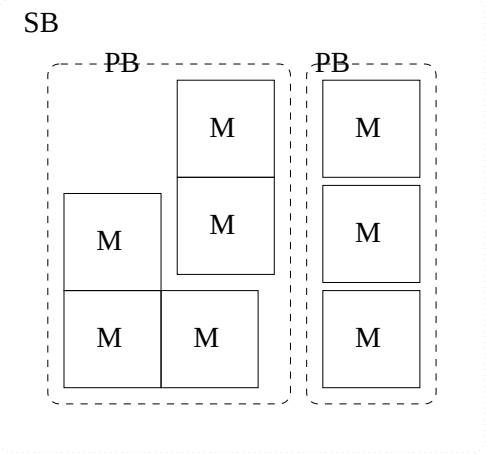

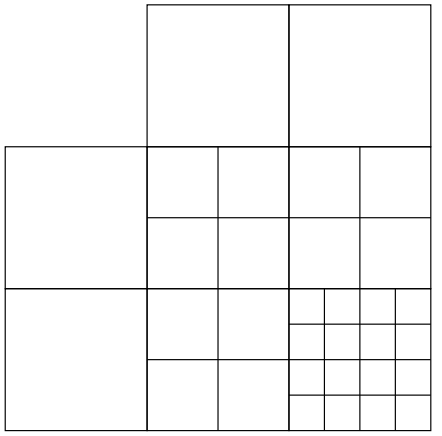

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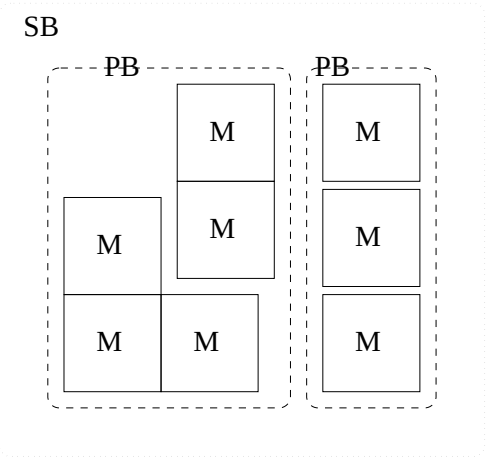

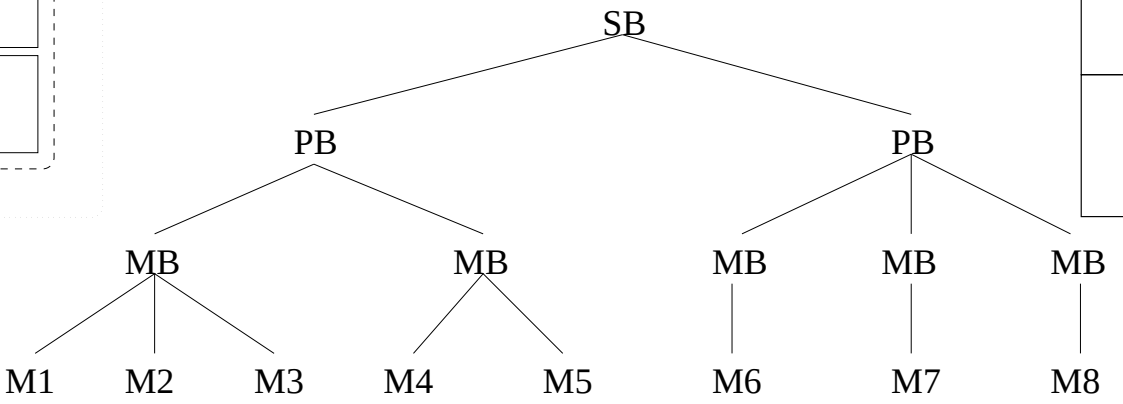

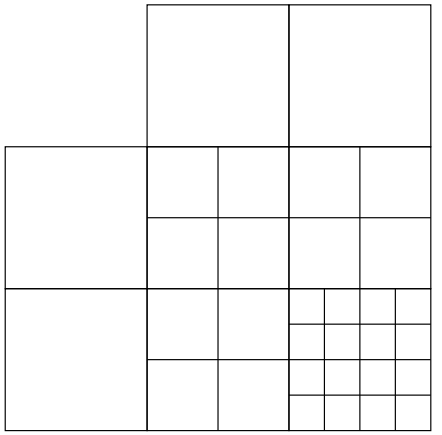

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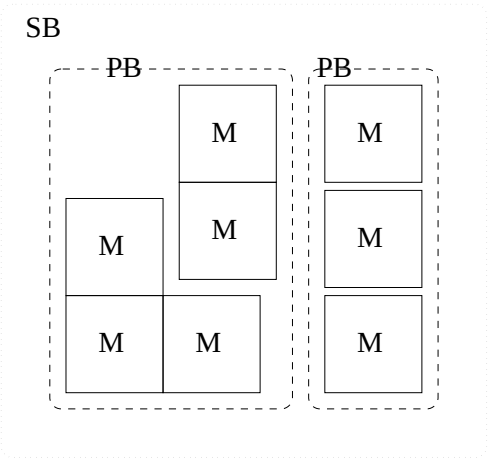

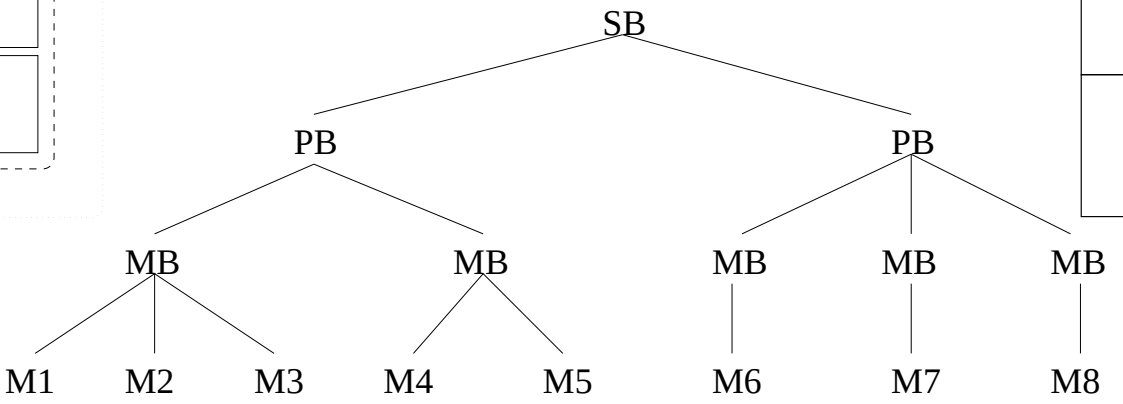

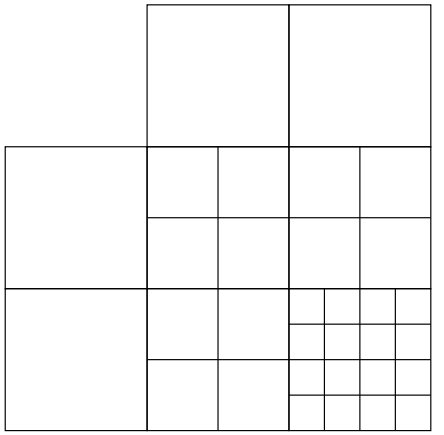

Structure parts: atomic units, matrix units, parallel units, subdomains, domain

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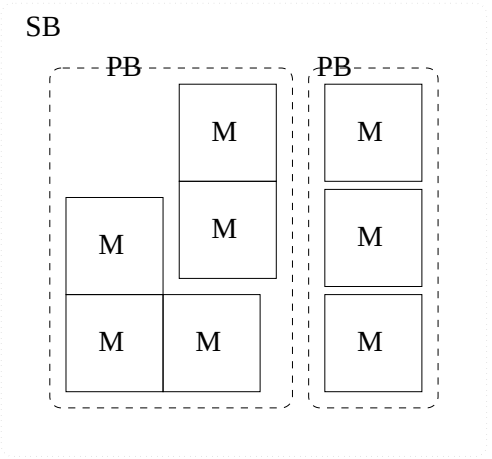

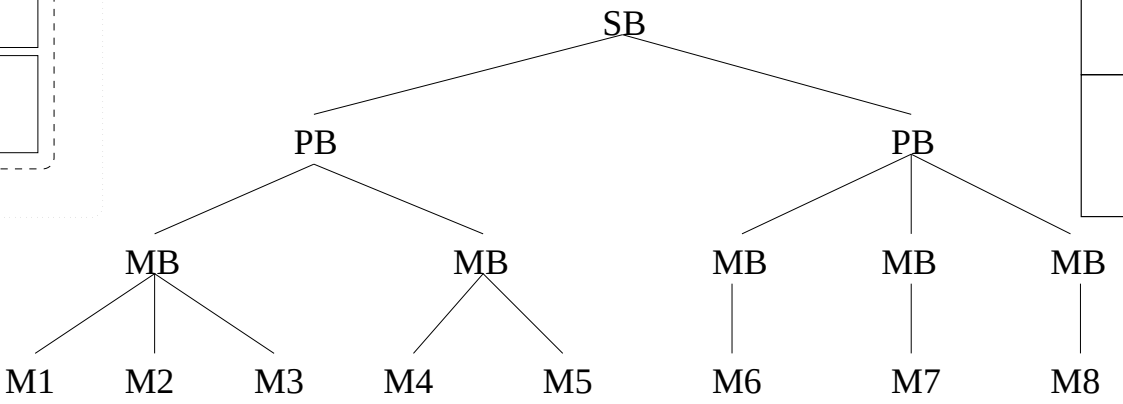

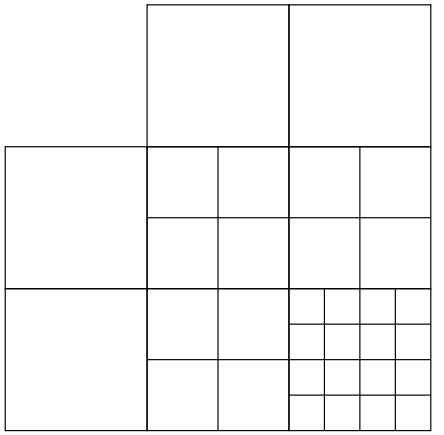

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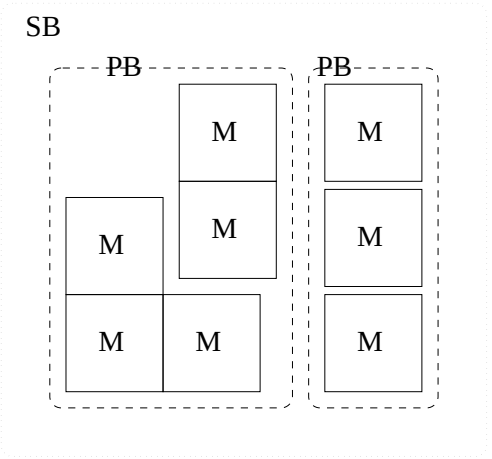

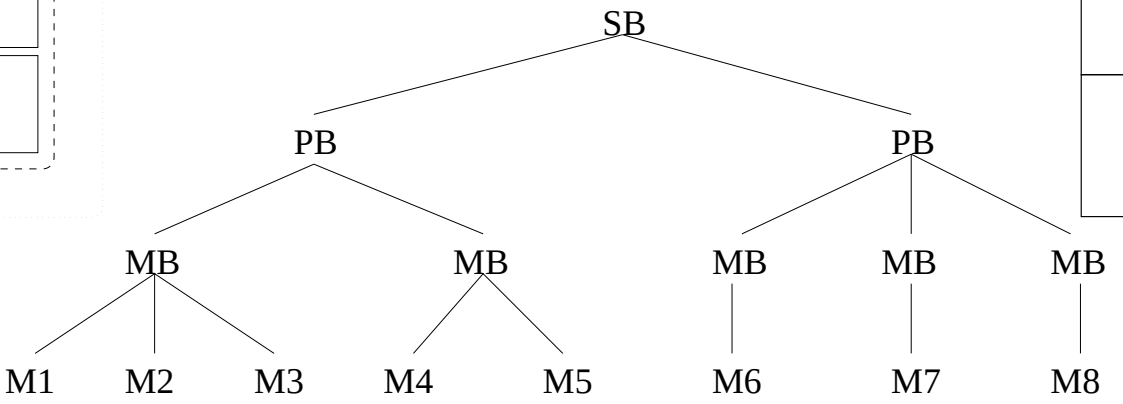

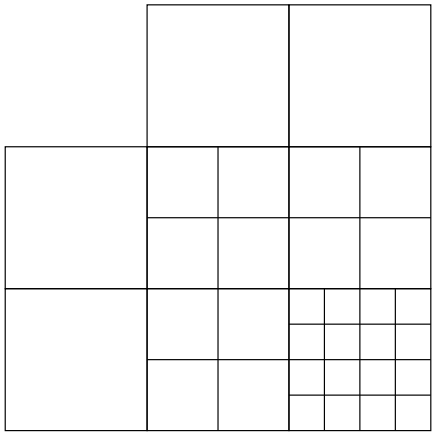

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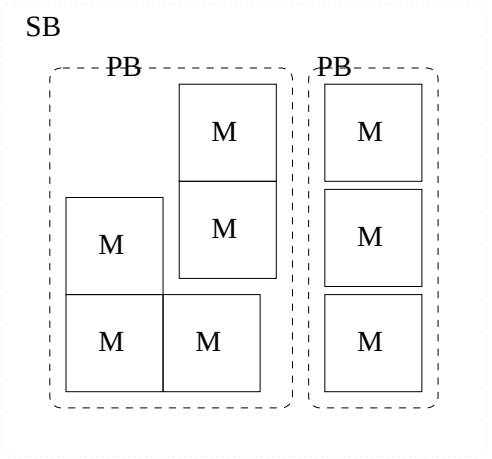

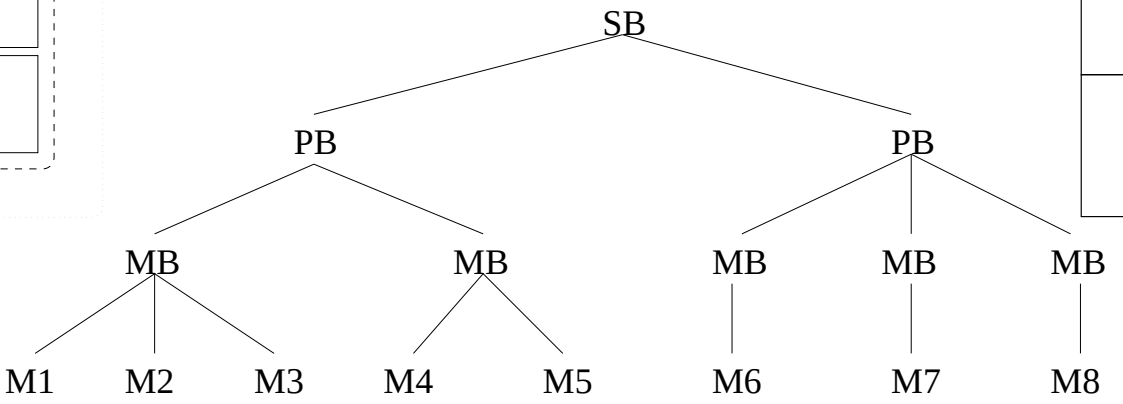

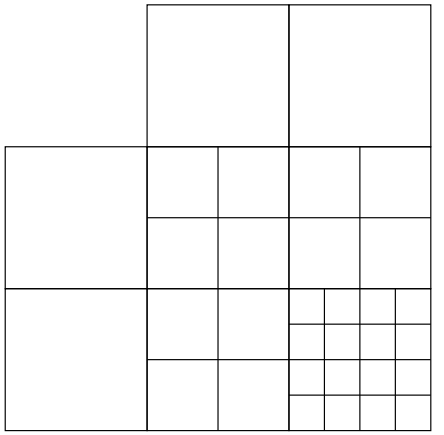

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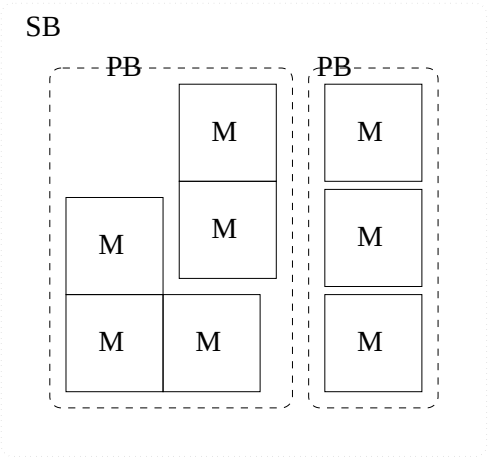

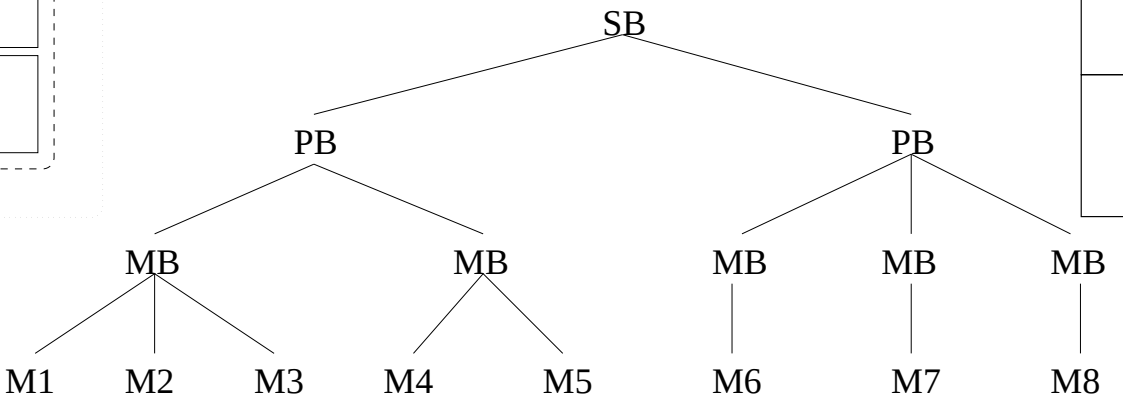

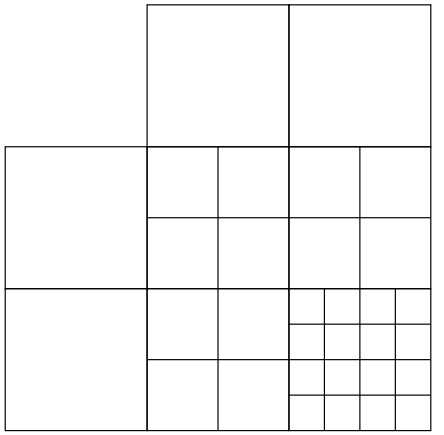

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Question: Corresponding solver?

Concepts for iterative parallel solvers

1. Standard multigrid

2. Standard Domain Decomposition

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   - parallelization of ’recursive’ smoothers only blockwise?

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$\Longrightarrow$ ScaRC (Scalable Recursive Clustering)

- Hide recursively alle anisotropies in more 'local' units (**robustness**)
- Perform most of Linear Algebra tasks on 'local' units (**efficiency**)

ScaRC (Scalable Recursive Clustering)

Standard multigrid with
(recursively defined)
block smoothers

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Standard multigrid with
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plus

Standard Domain Decomposition
with minimal overlap,
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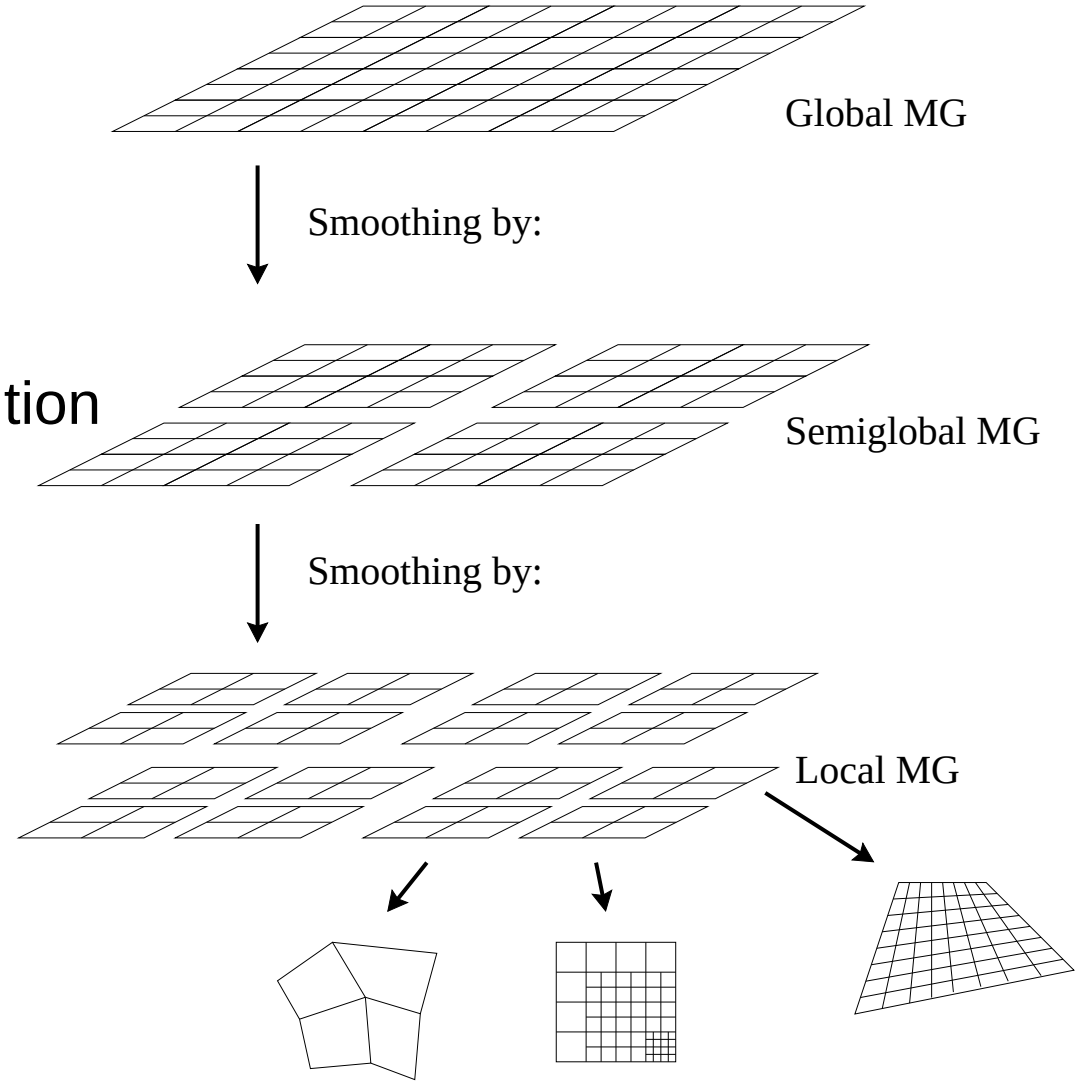
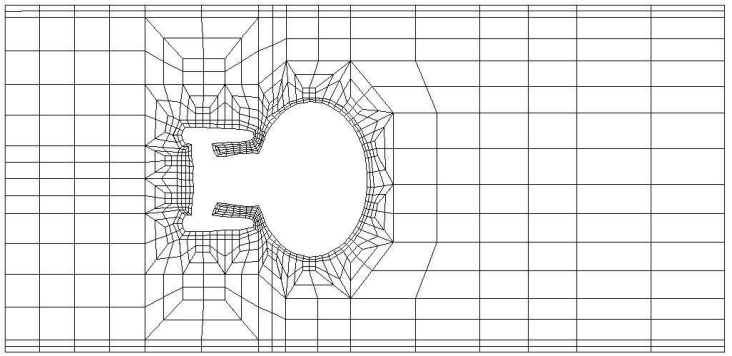


Example: Realization of ScaRC in FEAST

2D decomposition and zoomed (macro) element (LEVEL 3) with locally anisotropic refinement towards the wall



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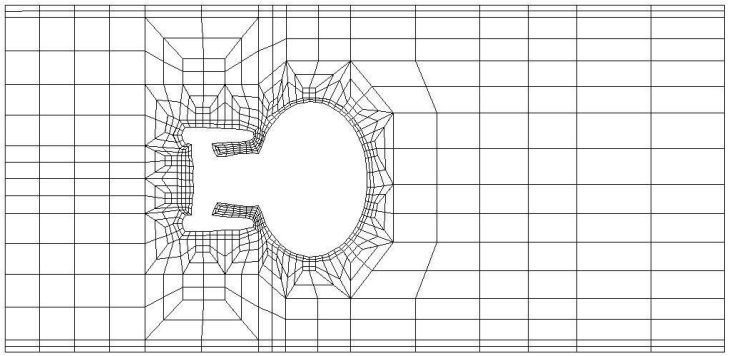

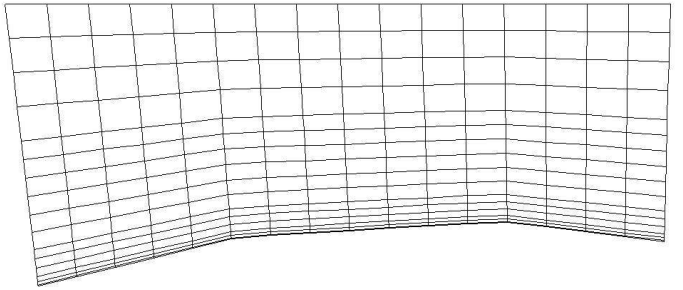

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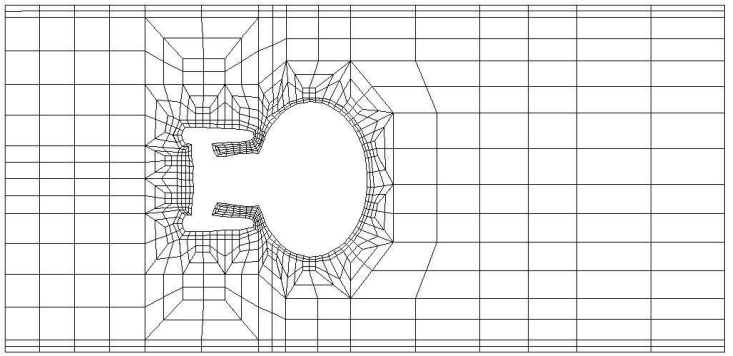

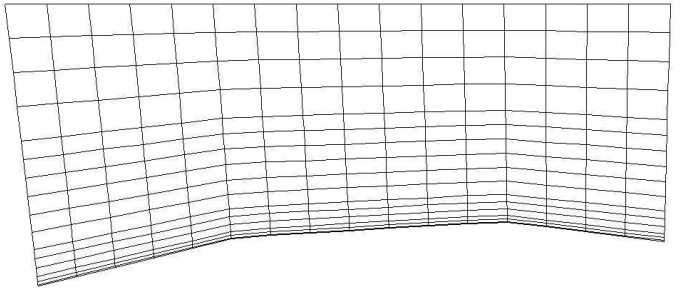

ScaRC-CG solver (smoothing steps: 1 global ScaRC ; 1 local ‘MG-TriGS’) for locally (an)isotropic refinement

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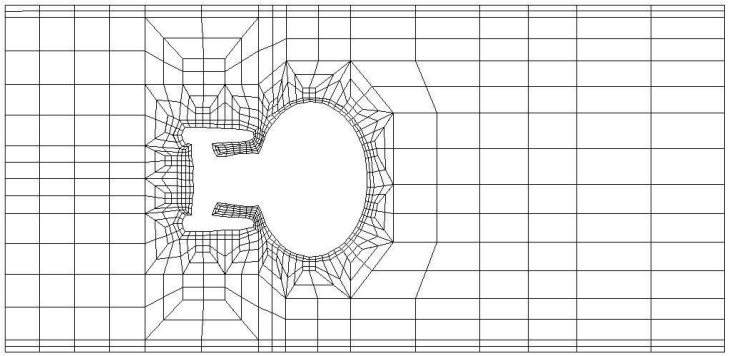
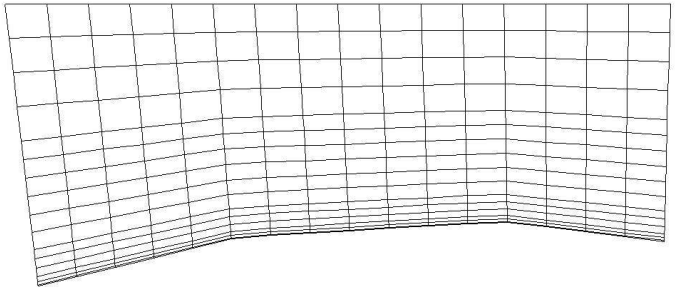




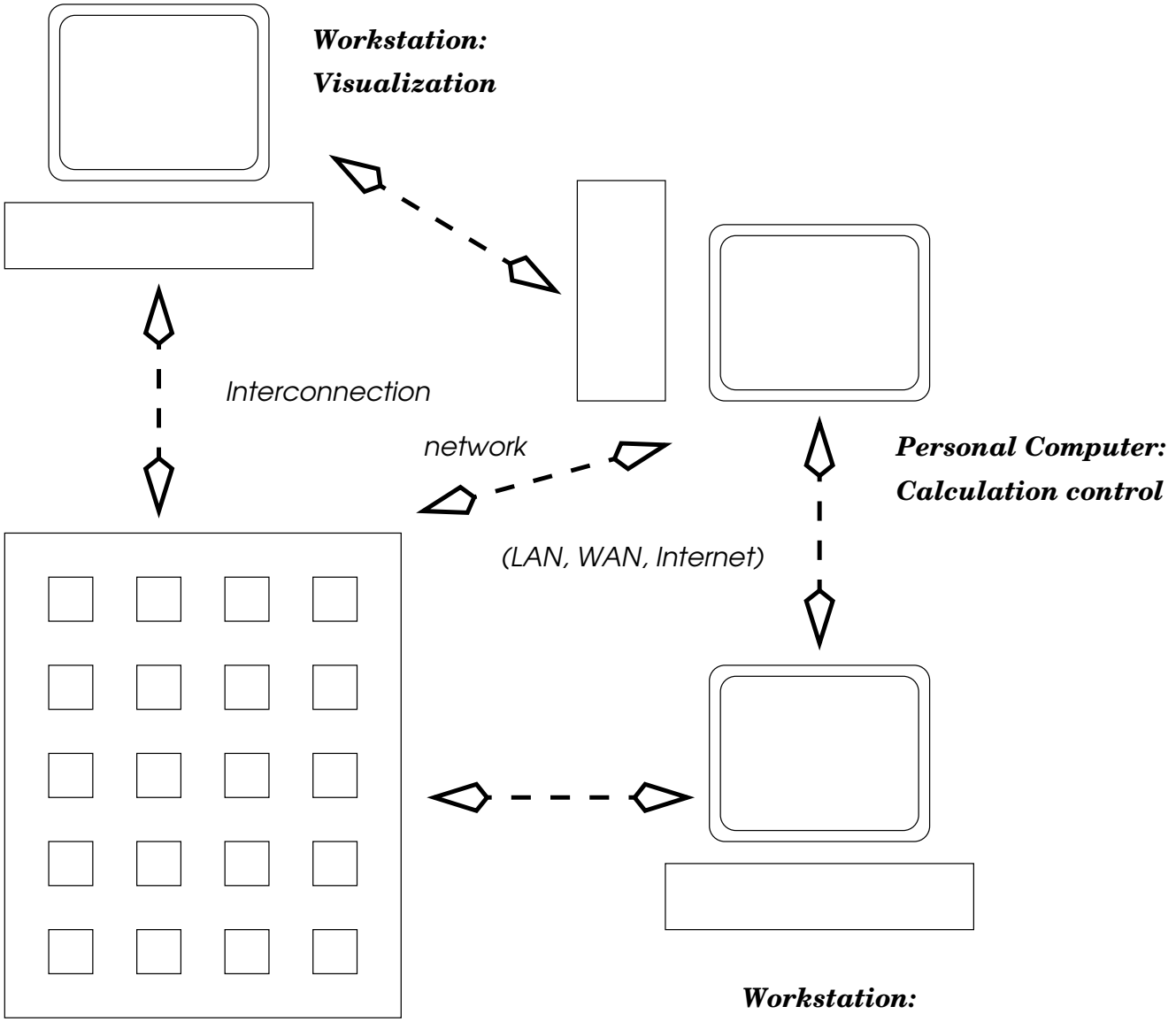
ScaRC-CG solver (smoothing steps: 1 global ScaRC ; 1 local 'MG-TriGS') for locally (an)isotropic refinement

Global (parallel) convergence rates

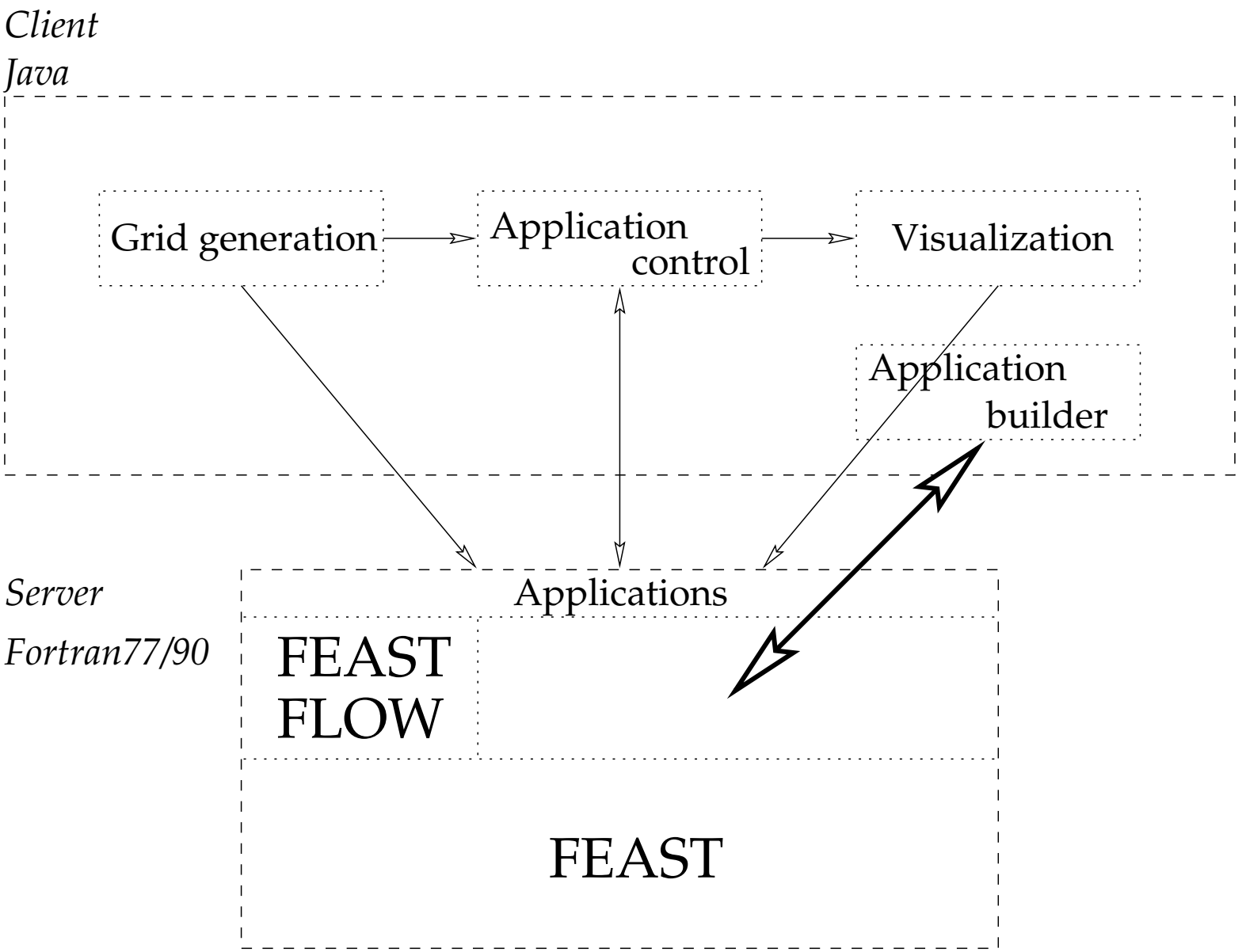
$\#NEQ$	Dirichlet 'Velocity'		Neumann 'Pressure'	
	$AR \approx 10$	$AR \approx 10^6$	$AR \approx 10$	$AR \approx 10^6$
$210,944$	0.17 (**8**)	0.18 (**8**)	0.21 (**9**)	0.15 (**8**)
$843,776$	0.17 (**8**)	0.17 (**8**)	0.20 (**9**)	0.17 (**8**)
$3,375,104$	0.18 (**9**)	0.19 (**9**)	0.22 (**10**)	0.22 (**10**)
$13,500,416$	0.19 (**9**)	0.18 (**9**)	0.23 (**10**)	0.23 (**10**)

FEAST structure

Overview


Workstation:
Visualization
Interconnection
network
(LAN, WAN, Internet)
Personal Computer:
Calculation control
Workstation:
Grid generation & editing
Parallel Computer:
Calculation

Overview


Client
Java
Grid generation
Application control
Visualization
Application builder
Server
Fortran77/90
Applications
FEAST
FLOW
FEAST

DeViSoRGrid 2D/3D

(**De**sign & **Vi**sualization **So**ftware **R**esource)

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DeViSoRControl I

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- adaption to existing solver FeatFlow, but also to further solvers with a universal description format with respect to menu structure and help system

DeViSoRControl II

universal protocol for communication with the numerical kernel

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- forwarding of grid geometries
- forwarding of solution vectors and values
- simulation control like tape recorder, forward, play, rewind, e.g. calculate 2 time steps, solution not satisfying, 3 time steps back, increase number of smoothing steps, continue calculation