Realistic Performance Evaluation of Numerical Simulations

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`http://gaia.iwr.uni-heidelberg.de/~ture`
`http://www.iwr.uni-heidelberg.de/~featflow`

Partners: **COMPAQ/DEC**, IBM, SUN, SGI, HP, etc.

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Soon: **Universität Dortmund**

We are in MA to celebrate:

- TOP 500: **TFlop/s computers** !!!
- **GFlop/s processors** in PC's/workstations !!!

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LINPACK $\sim$ Gaussian Elimination for **dense matrices**

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Reality for HPC in 'real life':

- Numerical simulations in CFD, Mechanics, QCD, etc.
- **Often:** Mesh-oriented discretization schemes (FEM, FD)

Sparse matrices !!!

Example I in 3D:

- $100 \times 100 \times 100$ grid points $\Longrightarrow$ **Problem size:** $N = 10^6$
- **Complexity of GE:** $N^{7/3} \approx 10^{14}$ FLOPs

100 sec on a 1 TFLOP/s computer

- **Complexity of MG:** $1,000N \approx 10^9$ FLOPs

100 sec on a 10 (!!!) MFLOP/s computer

Example II in 3D:

- $1,000^3$ grid points $\Longrightarrow$ **Problem size:** $N = 10^9$
- **Complexity of GE:** $N^{7/3} \approx 10^{21}$ FLOPs

10^6 **sec on a 1 P(!!!)FLOP/s computer**

- **Complexity of MG:** $1,000N \approx 10^{12}$ FLOPs

1,000 sec on a 1 (!!!) GFLOP/s computer

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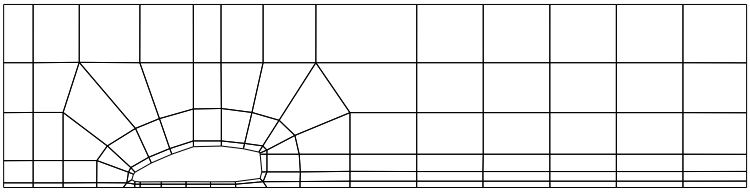
Modern Numerics !!!

- Discretization techniques
- **Iterative solvers** (Krylov-space, **MG**)

Results on general unstructured meshes

- SPARSE **MV** multiplication in **FEATFLOW** (F77 !!!)



Computer	#Unknowns	**CM**	**TL**	**STO**
	13,688	22	20	**19**
SUN E450	54,256	17	15	**13**
($\sim$ 250 MFLOP/s)	216,032	16	14	**6**
	862,144	16	15	**4**

- **STAR-CD**, **500,000 hexaeders** (by DaimlerChrysler)
- SGI Origin2000 (**6 processors**), **6.5 h** (CPU)

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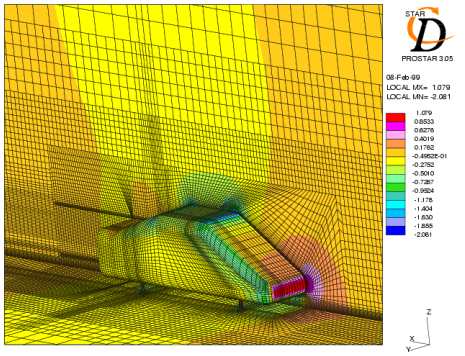
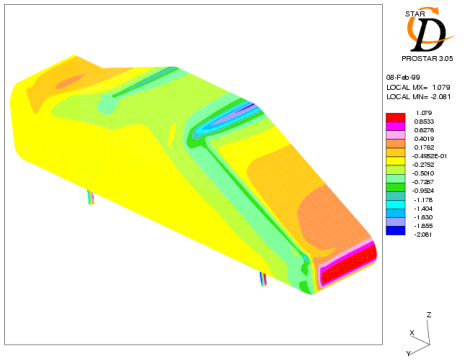
'Optimal' multigrid $\sim$ **0.1 sec/subproblem ???**

Quantity	**Experiment**	**Simulation**	**Difference**
Drag ('c_w')	0.165	0.317	**92 %**
Lift ('c_a')	-0.083	-0.127	**53 %**





Results on locally structured meshes

3D case	N	STO	SBB-V	SBB-C	**MG-V**	**MG-C**
DEC 21264	17^3	150	446	765	342	500
(500 MHz)	33^3	54	240	768	233	474
'**DS20**'	65^3	**24**	**249**	**713**	**196**	**447**
IBM RS6000/597	17^3	81	179	480	171	368
(160 MHz)	33^3	16	170	393	152	300
'**SP2**'	65^3	**8**	**178**	**393**	**150**	**276**
INTEL PII	17^3	28	56	183	48	136
(400 MHz)	33^3	24	53	139	47	116
'**ALDI**'	65^3	**19**	**54**	**125**	**45**	**101**

Sparse **MV techniques (STO)**

- MFLOP/s rates far away from '**Peak Performance**'
- Depending on **problem size + numbering**
- '**Old**' (IBM PWR2) partially **faster** then '**new**' (IBM P2SC)
- PC partially **faster** than processors in 'supercomputers' !!!

Feast **MV techniques (SBB)**

- 'Supercomputing' power gets visible (up to **800 MFLOP/s**)
- **Warning:** Hard work !!!

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Processors are 'sensible' Parallel-Vector supercomputers w.r.t. **caching-in + pipelining**

FEAST project

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Numerics and **implementation** techniques adapted to **hardware !!!**

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Precise knowledge of **processor** characteristics

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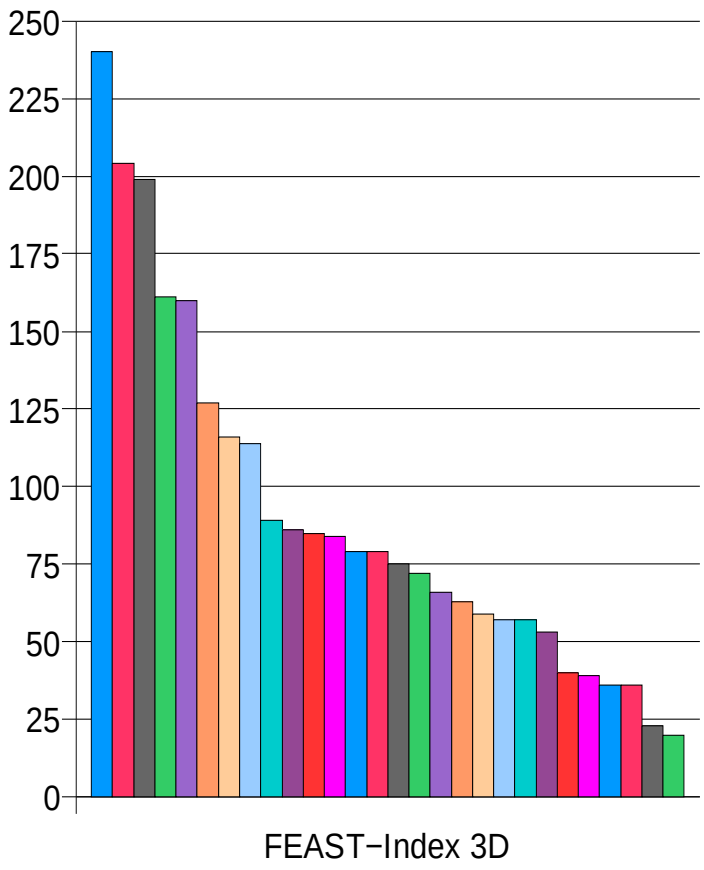
(Collection of) **FEAST INDICES**



Results for the different **tasks in MG** for various **FEM** discretizations and **mesh sizes**

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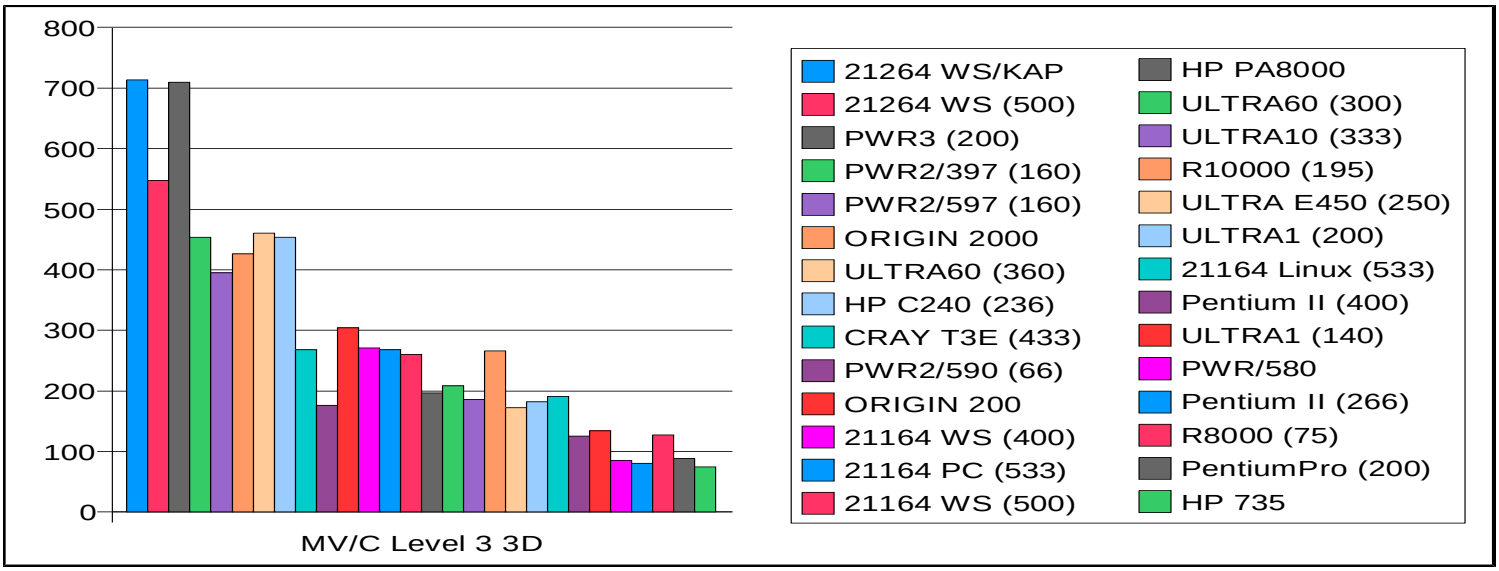
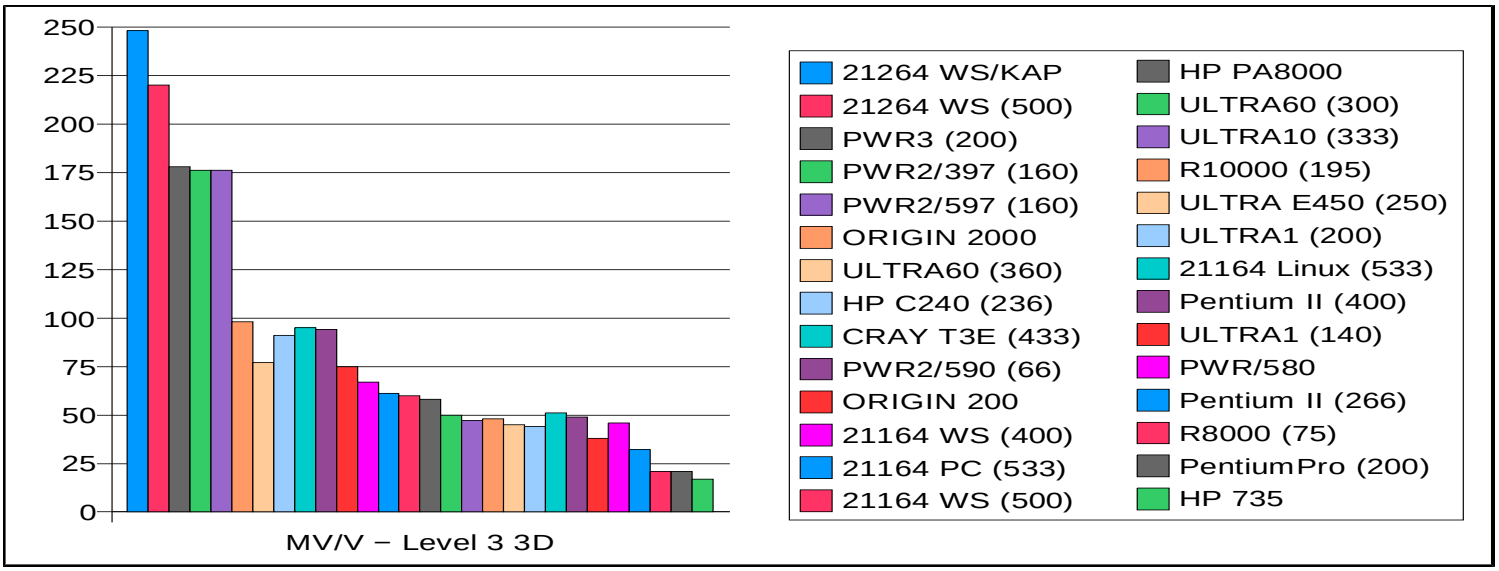
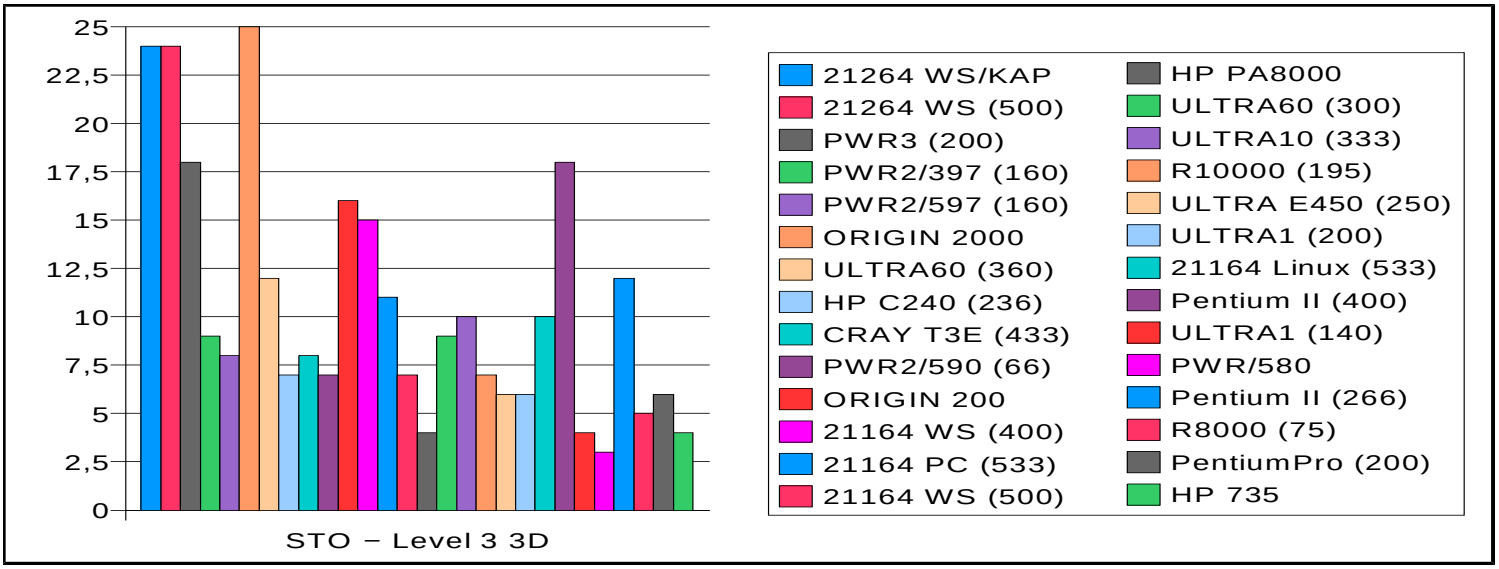
Many FEAST (sub)indices

MV-MULT with identical matrix !!!







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Future of High Performance Computing:

Numerics *and* **implementation** *techniques and* **hardware** *developments massively influence each others !!!*

Mathematicians, computer scientists and processor developers have to **come together !!!**

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Otherwise: **Buy INTEL PC's ...**

Desired cooperation:

- Processor testing (**FEAST INDICES, FEATFLOW**)
- 'Hand-coded' **SBBLAS** for FEM discretizations
- Tuning of massively parallel and vectorized **FEAST** software