

Teaching High Performance Computing to Scientists and Engineers: A Model-Based Approach

Georg Hager, Jan Treibig, Gerhard Wellein
Erlangen Regional Computing Center (RRZE)
University of Erlangen-Nuremberg
Germany

A little history of our group: HPC@RRZE



1998: First HPC consultant at RRZE

2000: Project KONWIHR – one additional consultant

2002: Two additional KONWIHR consultants

2003: First permanent position in the group

2008: Second permanent position, two PhD students

2011: Spin-off company

**Today: One professor, three permanent positions,
one postdoc, four PhD students, >90 publications**

1 computer scientist

Consulting



Chemistry

Physics

Engineering

HPC@RRZE

Materials
Science

Applied
Math

Computer
Science

Teaching activities



Supercomputing
Tutorial “Hybrid
MPI/OpenMP”

Supercomputing
Tutorial “Multicore
Optimization”

HPC@RRZE

Textbook
“Introduction to
High Performance
Computing for
Scientists and
Engineers”

Lecture
“Programming
Techniques for
Supercomputers”

Course “Parallel
Programming of
High Performance
Systems”

Textbook

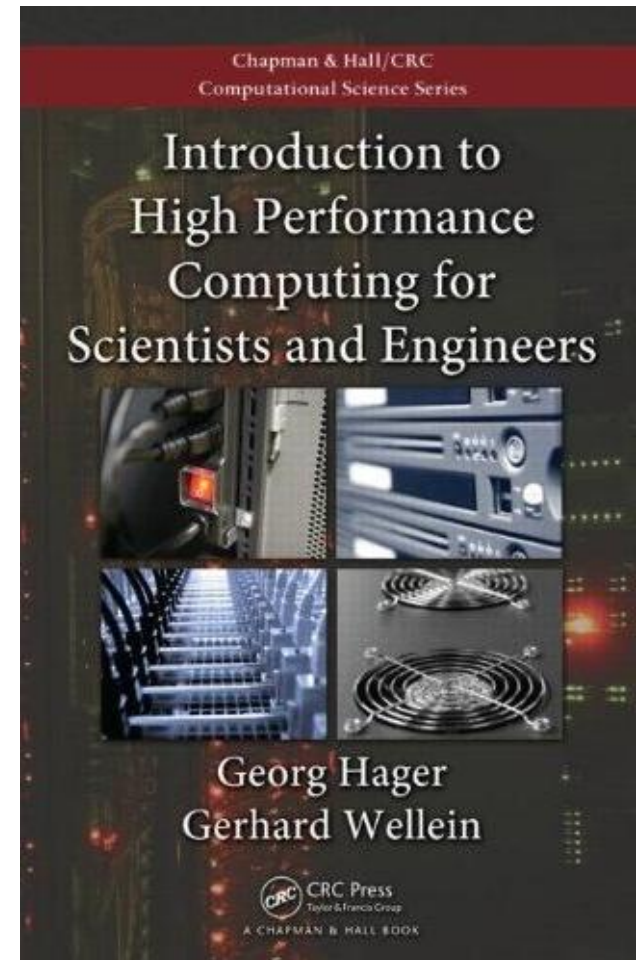


Georg Hager and Gerhard Wellein:
**Introduction to High Performance
Computing for Scientists and Engineers**

CRC Press, ISBN 978-1439811924

356 pages

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Model building



How do scientists write numerical software?



The premises



1. Parallelism necessary but not sufficient
2. Efficient use of resources is key
3. I have to know when to stop optimizing (the “good enough” point)

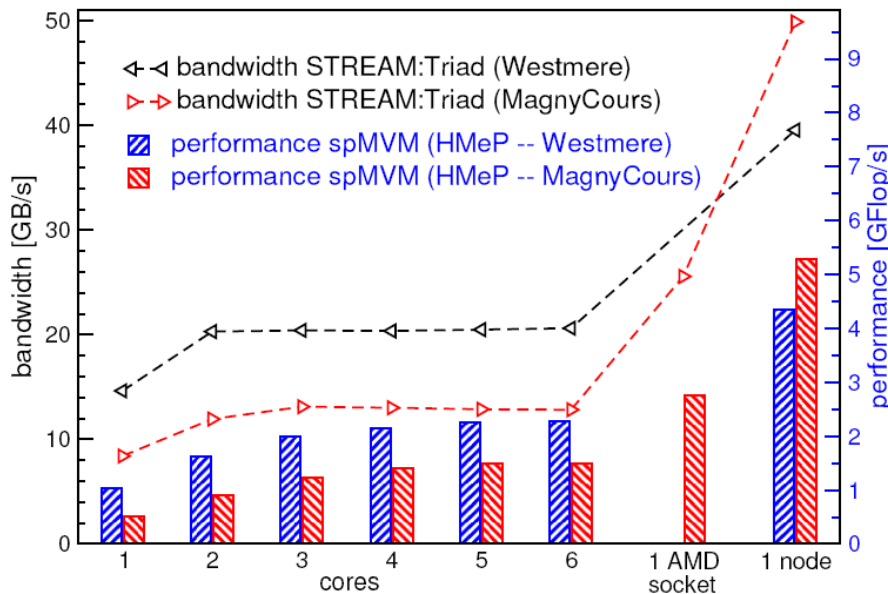
Consequence:

Performance modeling guides the way!

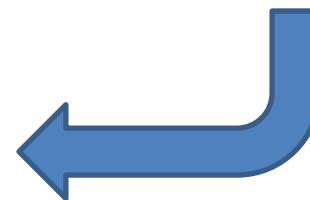
Example: CRS Sparse Matrix-Vector Multiply

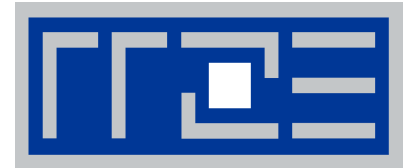


```
do i = 1, Nr
  do j = row_ptr(i), row_ptr(i+1) - 1
    C(i) = C(i) + val(j) * B(col_idx(j))
  enddo
enddo
```



$$\begin{aligned}
 B_{\text{CRS}} &= \left(\frac{12 + 24/N_{\text{nzr}} + \kappa}{2} \right) \frac{\text{bytes}}{\text{flop}} \\
 &= \left(6 + \frac{12}{N_{\text{nzr}}} + \frac{\kappa}{2} \right) \frac{\text{bytes}}{\text{flop}} .
 \end{aligned}$$





Federal Ministry
of Education
and Research

THANK YOU.

