

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

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# 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

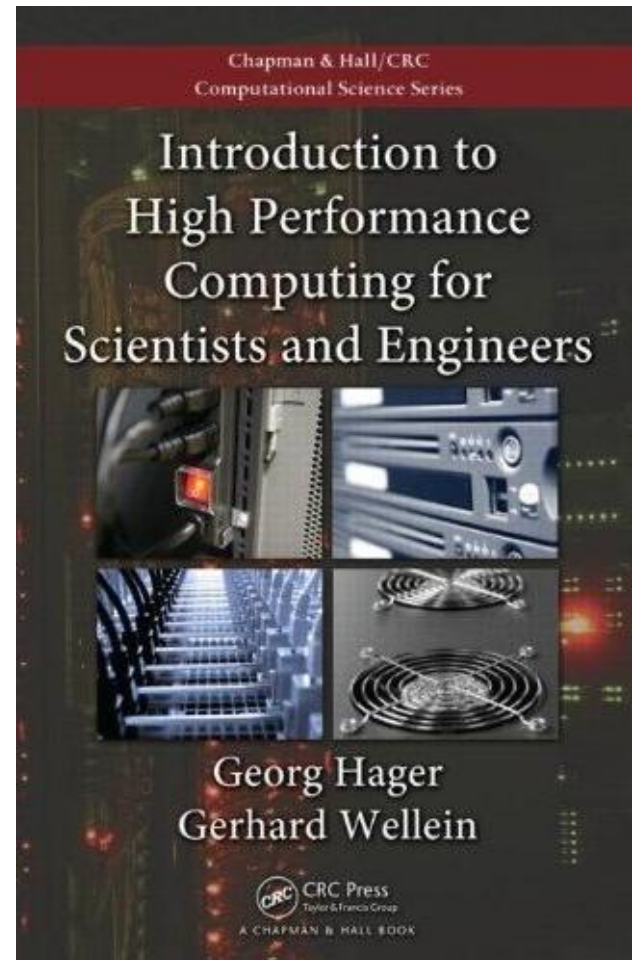


*Georg Hager and Gerhard Wellein:*  
**Introduction to High Performance  
Computing for Scientists and Engineers**

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:

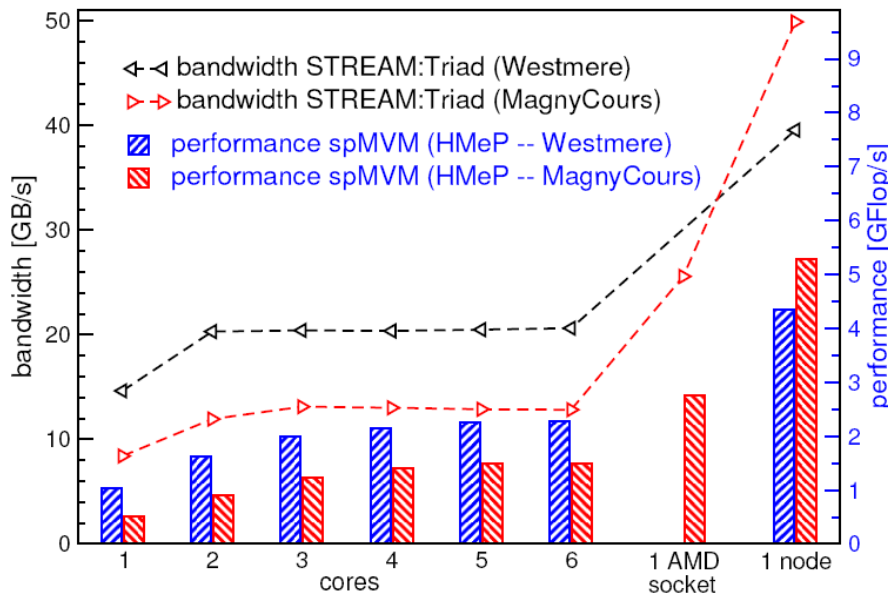
**Performance modeling guides the way!**

# Example:

## CRS Sparse Matrix-Vector Multiply

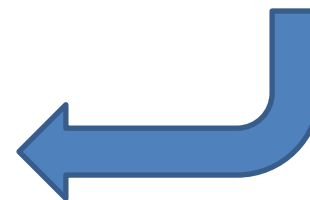


```
do i = 1, Nr
  do j = row_ptr(i), row_ptr(i+1) - 1
    C(i) = C(i) + val(j) * B(col_idx(j))
  enddo
enddo
```

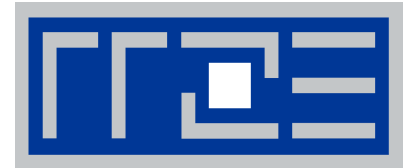


$$B_{\text{CRS}} = \left( \frac{12 + 24/N_{\text{nzr}} + \kappa}{2} \right) \frac{\text{bytes}}{\text{flop}}$$

$$= \left( 6 + \frac{12}{N_{\text{nzr}}} + \frac{\kappa}{2} \right) \frac{\text{bytes}}{\text{flop}} .$$







Federal Ministry  
of Education  
and Research

**THANK YOU.**

