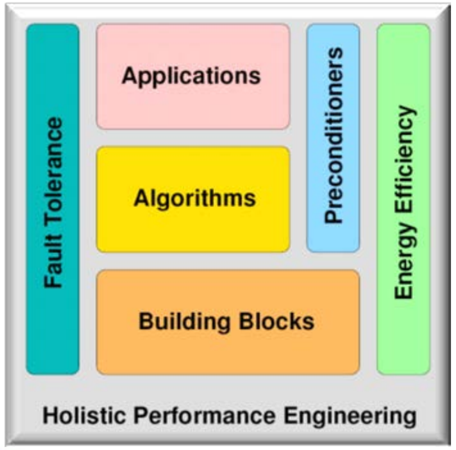
SPPEXA

DFG Projekt ESSEX



A Software Infrastructure for Solving Quantum Physics Problems on Extremely Parallel Systems

Achim Basermann, Jonas Thies, Melven Röhrig-Zöllner
German Aerospace Center (DLR)
Simulation and Software Technology
Department High-Performance Computing
Linder Höhe, Cologne, Germany

DLR

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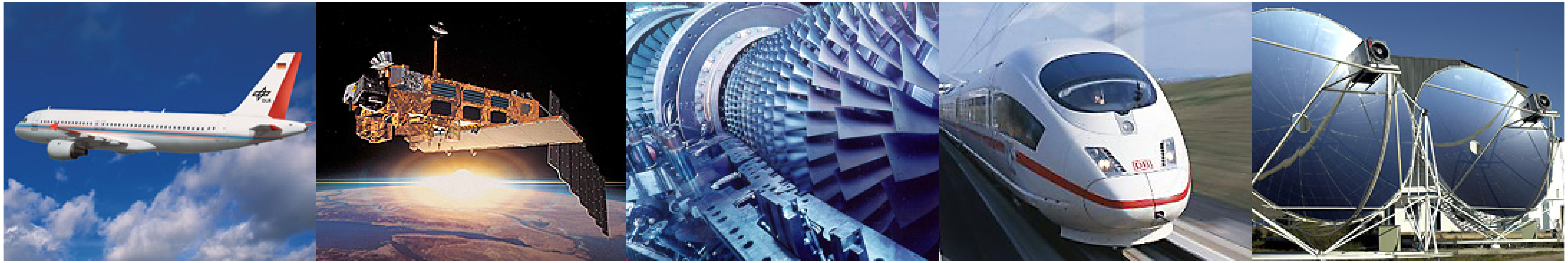


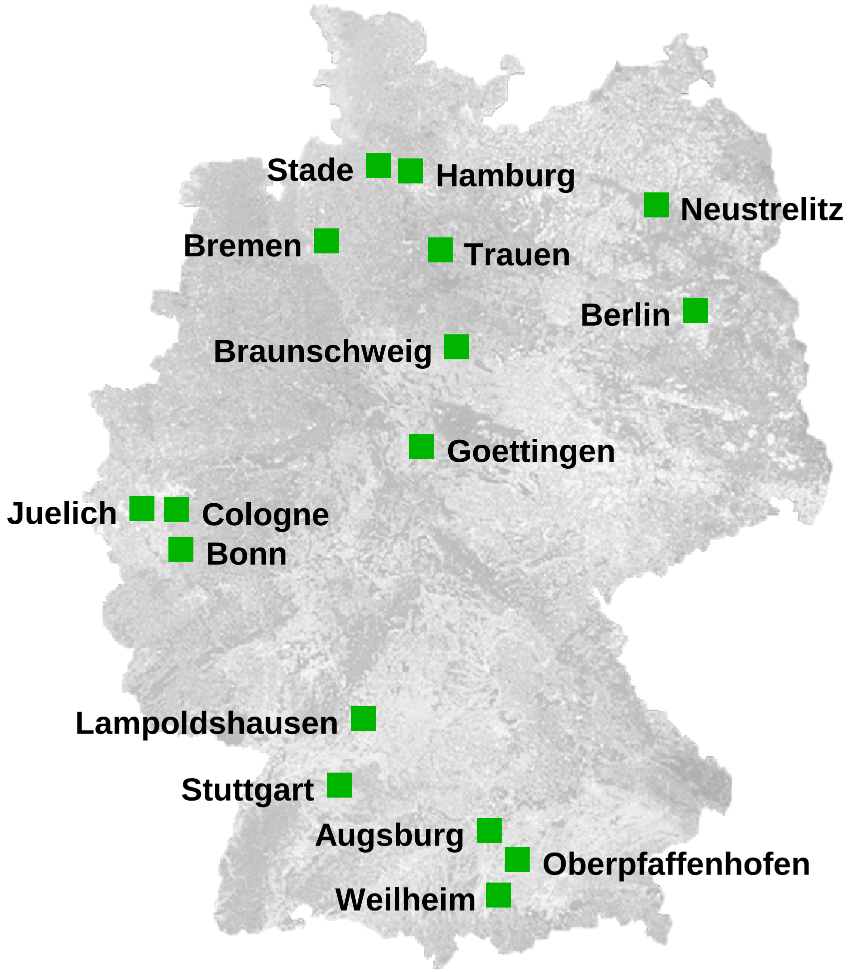
- Research Institution
- Space Agency
- Project Management Agency

DLR Locations and Employees

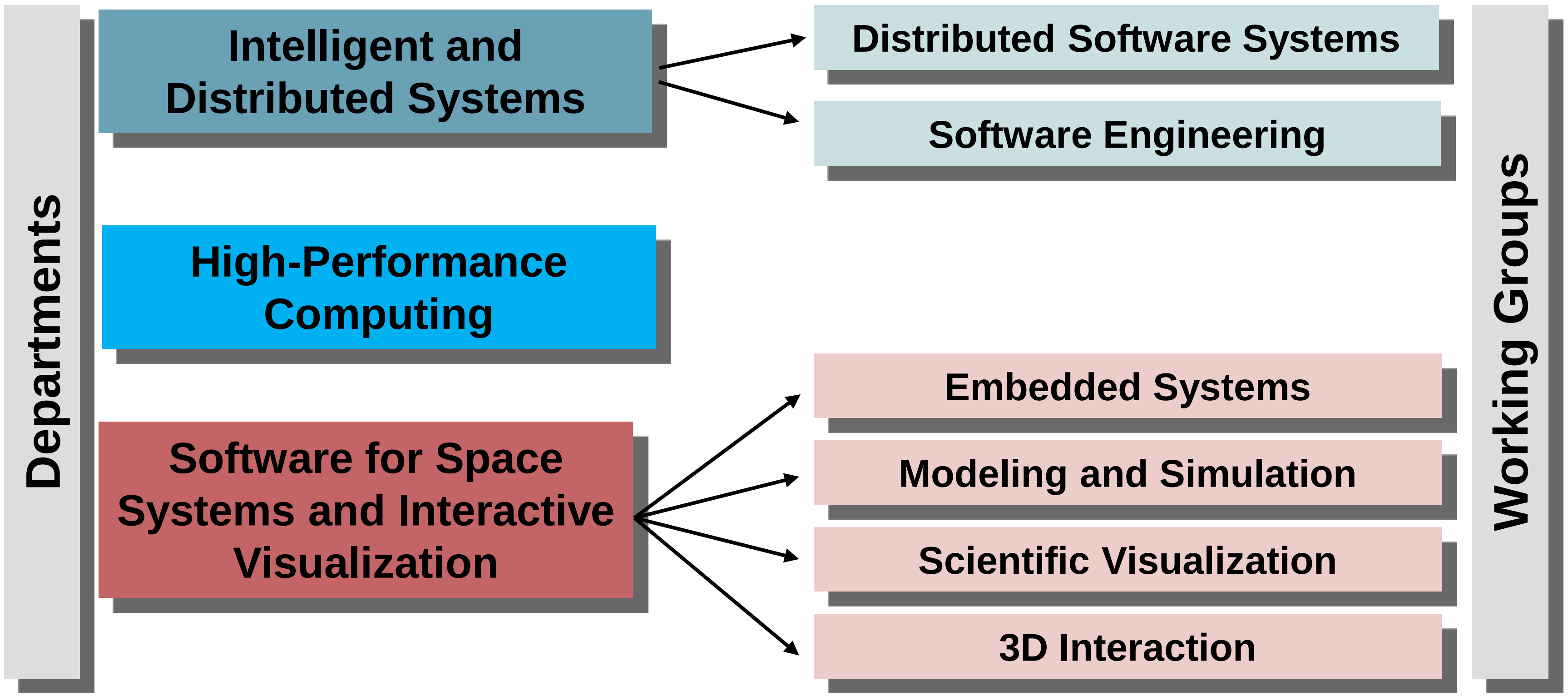
Approx. 8000 employees across 33 institutes and facilities at

- 16 sites.

Offices in Brussels, Paris, Tokyo and Washington.



DLR Institute Simulation and Software Technology
Scientific Themes and Working Groups



Survey

- ESSEX motivation
- The ESSEX software infrastructure
- Holistic view: application, algorithm and performance
- Conclusions
- Future work

ESSEX Motivation: Requirements for Exascale

Hardware
Fault tolerance
Energy efficiency
New levels of parallelism

Quantum Physics Applications
Extremely large sparse matrices:
eigenvalues, spectral properties,
time evolution

ESSEX

Exascale Sparse Solver Repository (ESSR)
ghost / PHIST

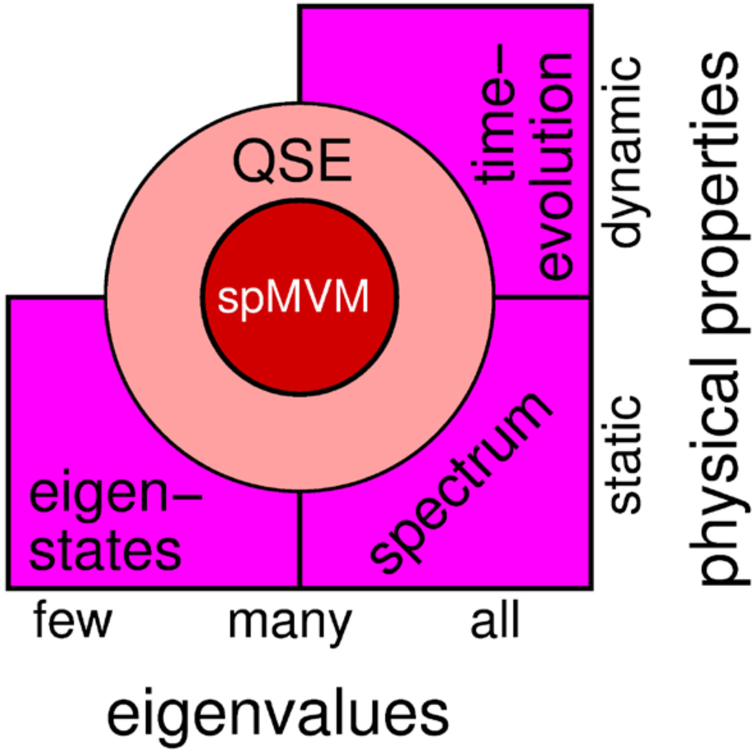
- FT concepts, programming for extreme parallelism
- Sparse eigensolvers, preconditioners, spectral methods
- Quantum physics / chemistry
- ESSEX applications: Graphene, topological insulators, …

ESSEX: Physical Motivation and Sparse Eigenvalue problem

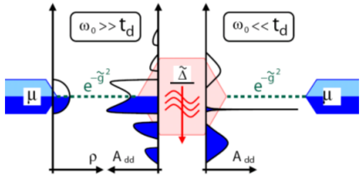
Solve large sparse eigenvalue problem

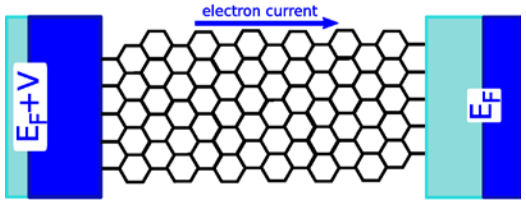
$$\boldsymbol{H}\,\boldsymbol{x} = \boldsymbol{\lambda}\,\boldsymbol{x}$$

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t)$$



$(\boldsymbol{\lambda_i}, \mathbf{x_i})$





ESSEX Software Development: Basics

- **Git** for distributed software developement
- **Merge-request workflo**w for code review; changes only in branches
- Own MPI extension for **Google Test**
- Realization of **continuous-integratio**n with Jenkins server

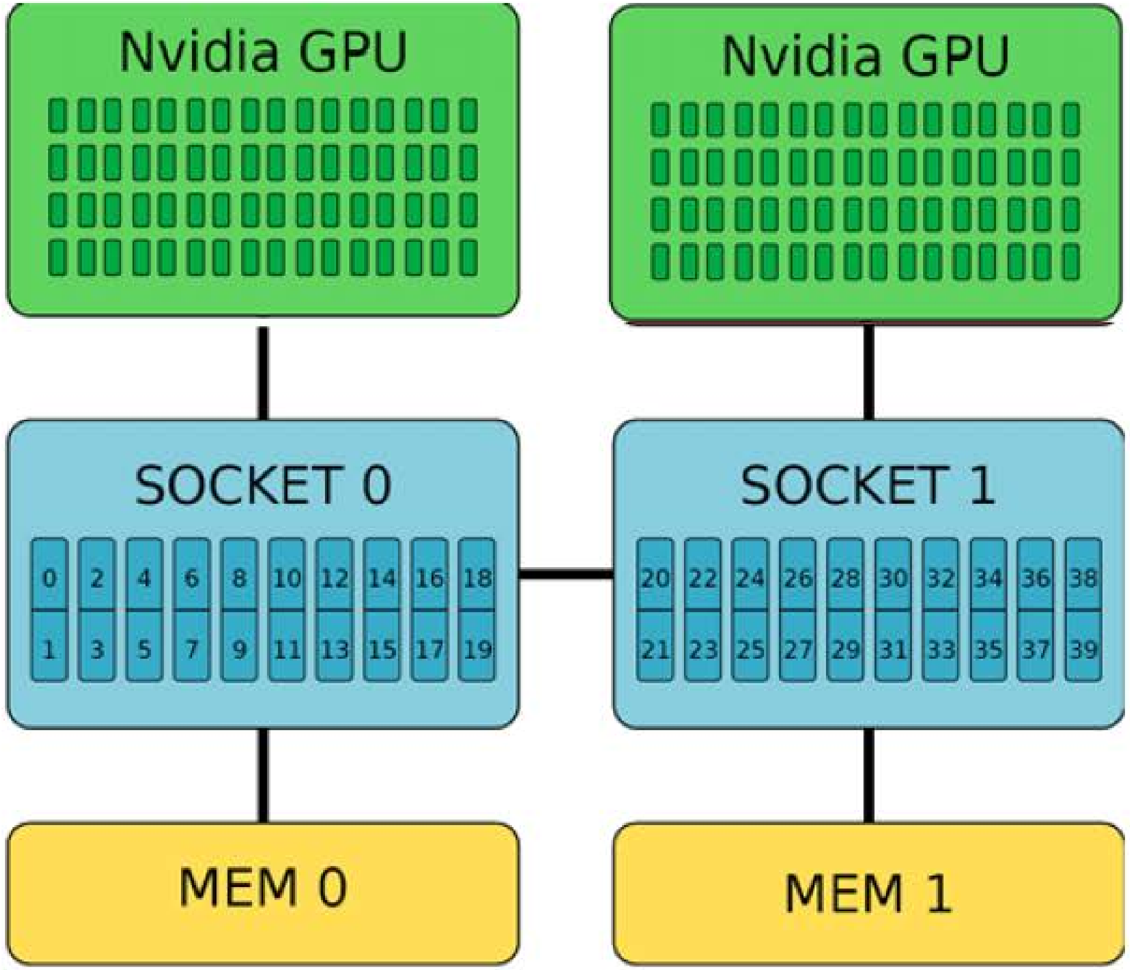
The ESSEX Software Infrastructure: Kernel Library GHOST

(General Hybrid and Optimized Sparse Toolkit) provides

- intelligent resource management for heterogenous systems
  - automatic pinning of threads to cores
  - asynchronous execution of (larger) tasks
- some fully optimized kernels for sparse matrix methods
  - sparse matrix-(multi)vector multiplication (spM(M)VM)
  - 'tall and skinny' matrices in row or column major ordering
- target platforms right now: Intel CPUs, Xeon Phi and Nvidia GPUs
- programming model: 'MPI+X',
  with X=SIMD intrinsics, OpenMP and CUDA

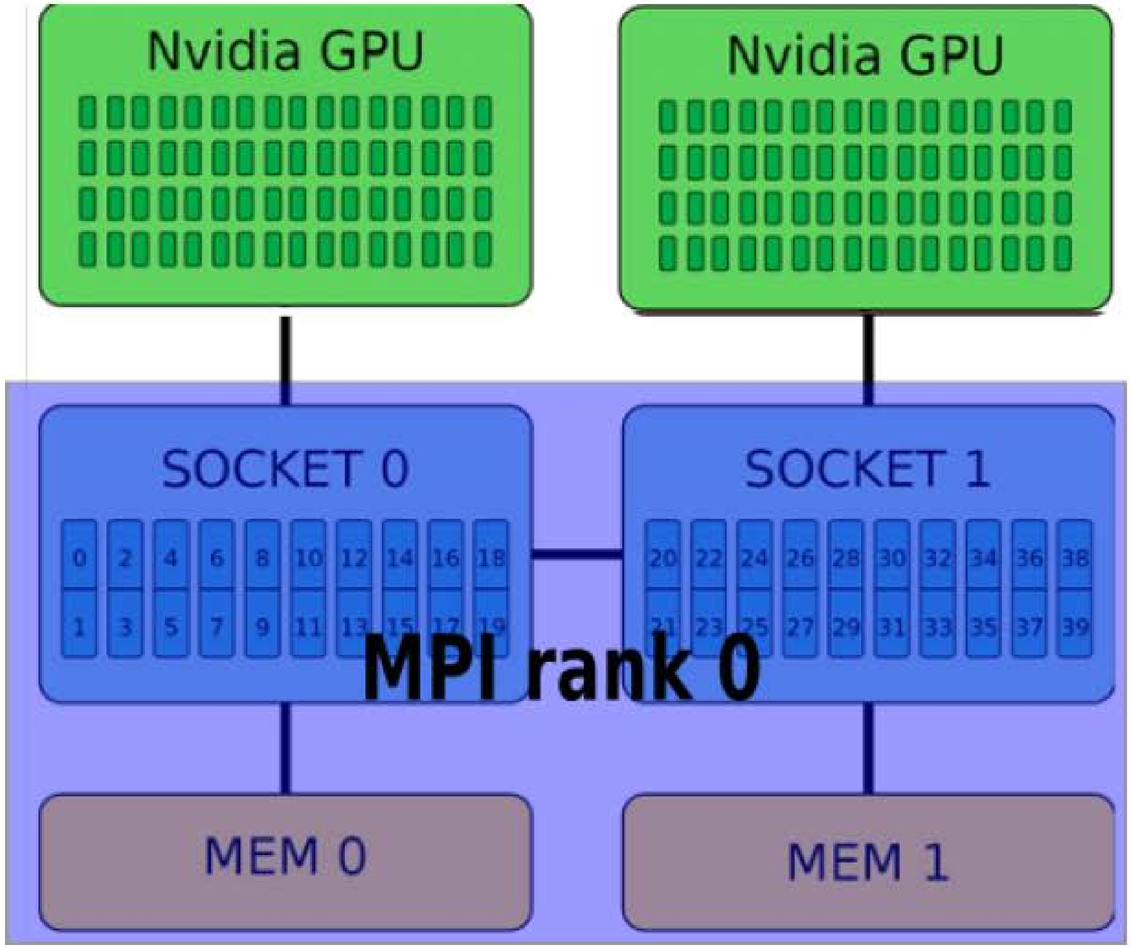
The ESSEX Software Infrastructure: MPI + X with GHOST

- System with multiple CPUs (NUMA domains) and GPUs



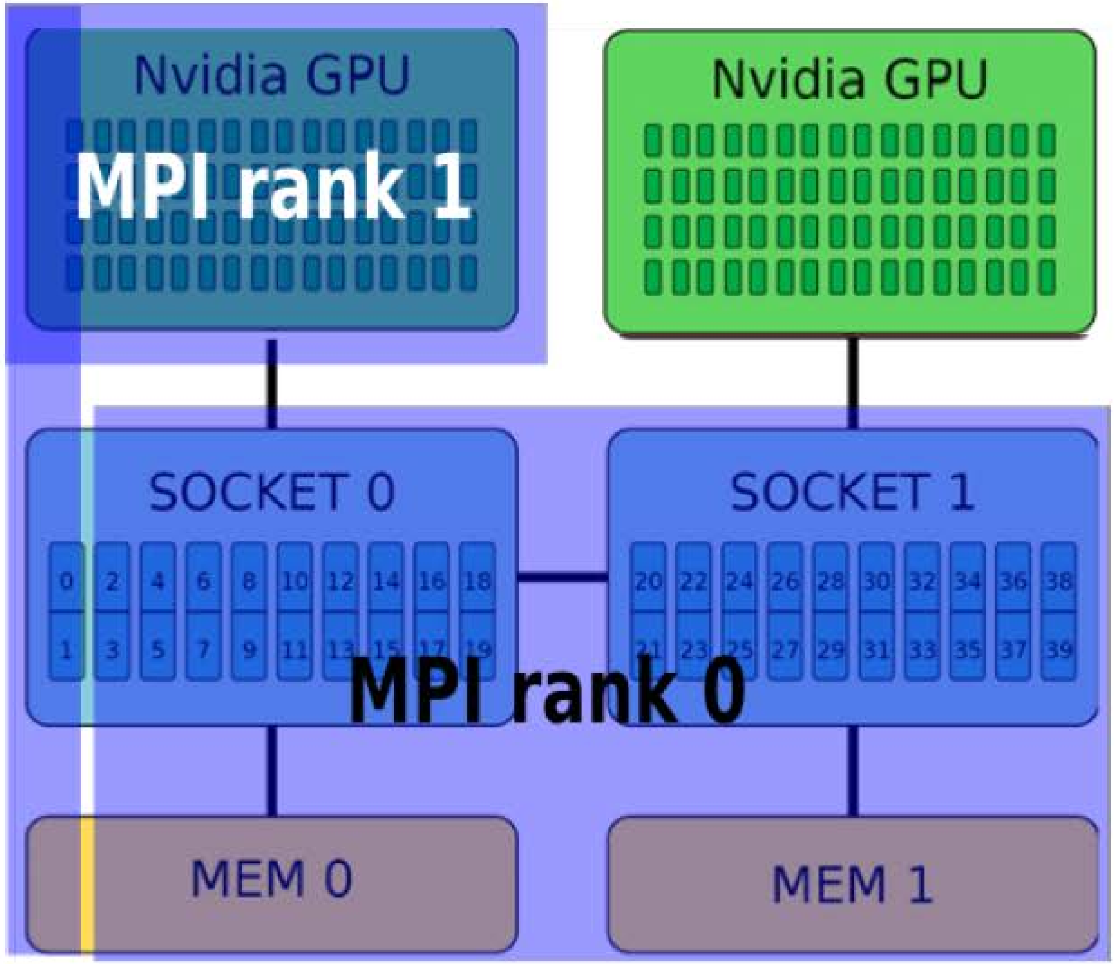
The ESSEX Software Infrastructure: MPI + X with GHOST

- System with multiple CPUs (NUMA domains) and GPUs
- -np 1: use entire CPU



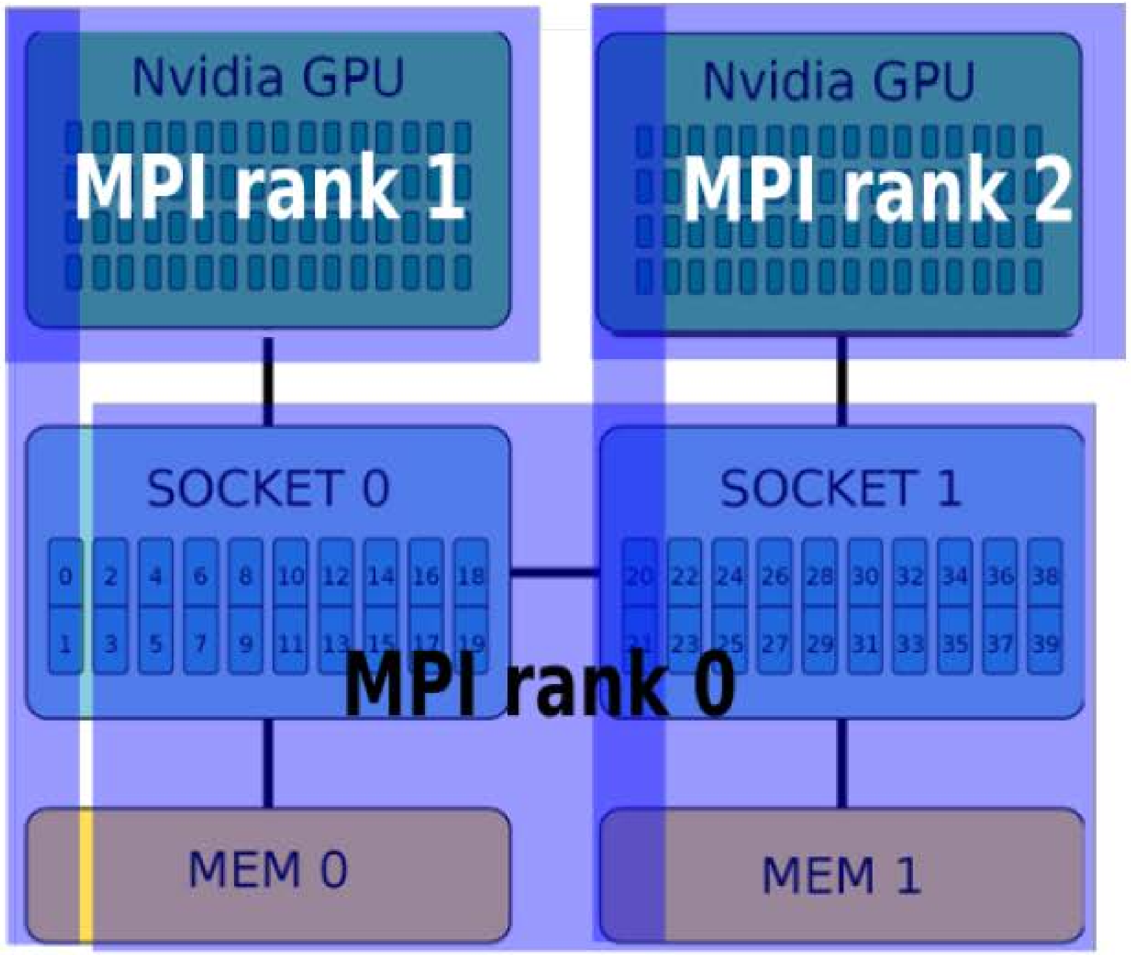
The ESSEX Software Infrastructure: MPI + X with GHOST

- System with multiple CPUs (NUMA domains) and GPUs
- -np 1: use entire CPU
- -np 2: use CPU and first GPU



The ESSEX Software Infrastructure: MPI + X with GHOST

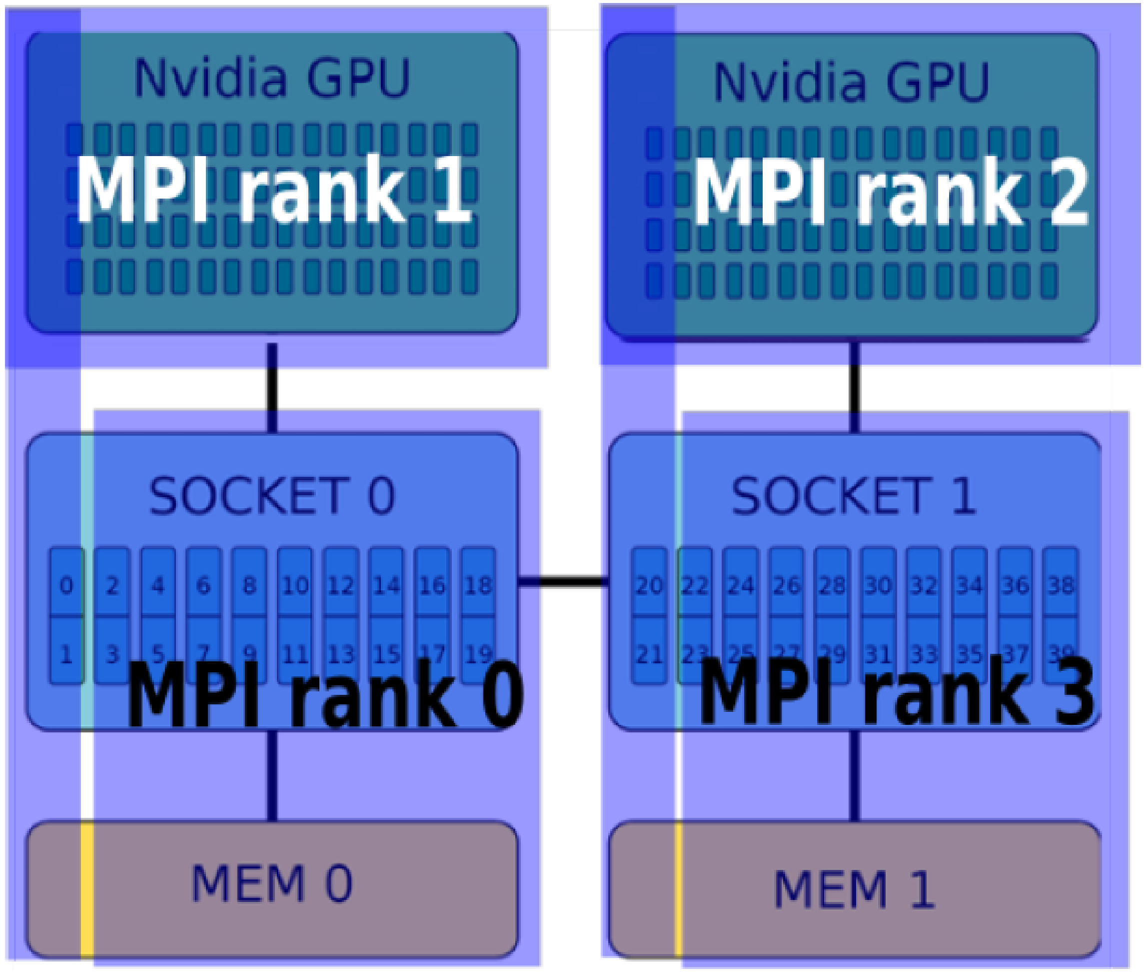
- System with multiple CPUs (NUMA domains) and GPUs
- -np 1: use entire CPU
- -np 2: use CPU and first GPU
- -np 3: use CPU and both GPUs



The ESSEX Software Infrastructure: MPI + X with GHOST

- System with multiple CPUs (NUMA domains) and GPUs
- -np 1: use entire CPU
- -np 2: use CPU and first GPU
- -np 3: use CPU and both GPUs
- -np 4: use one process per socket and one for each GPU

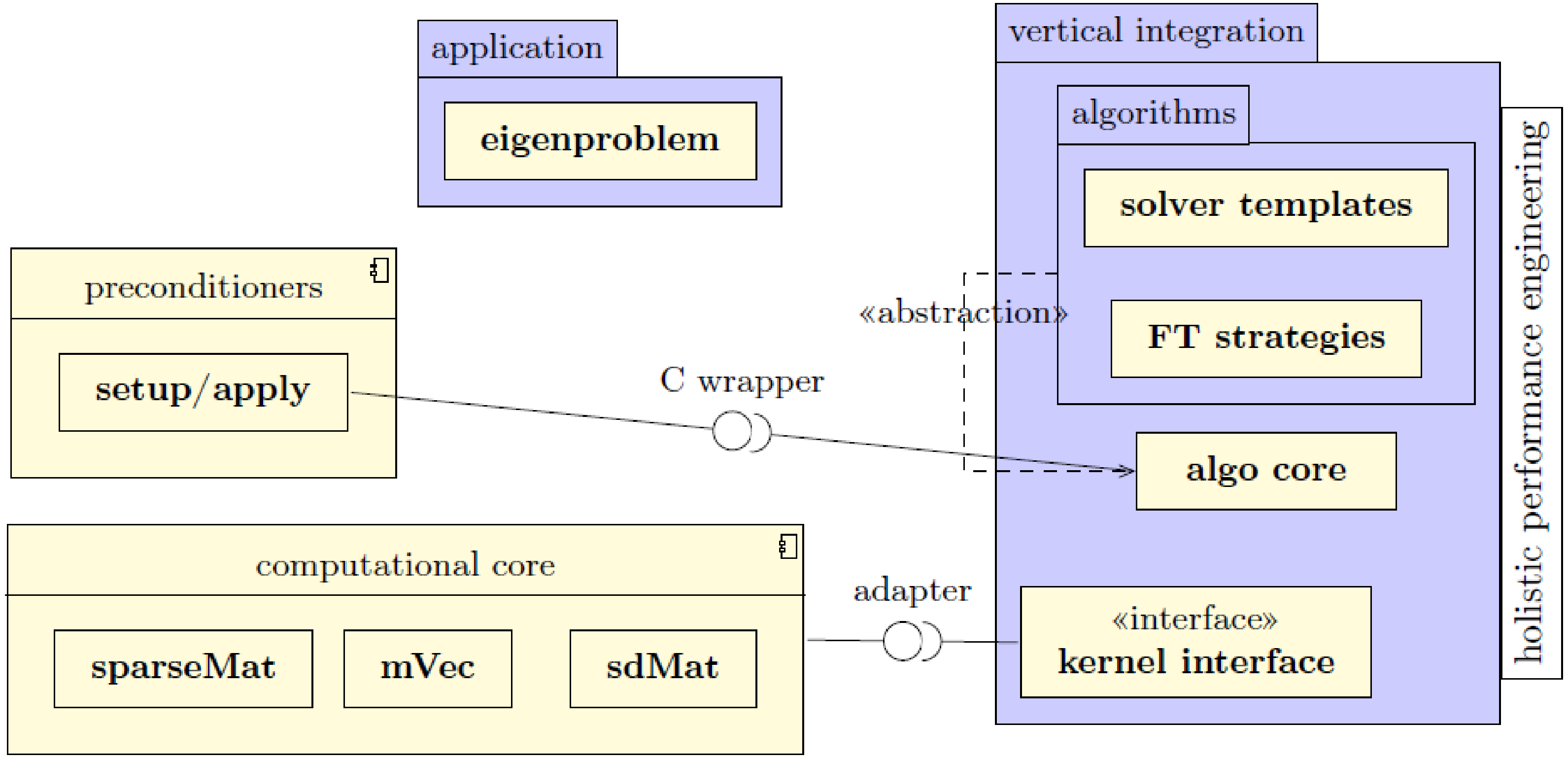
Option: distribute problem according to memory bandwidth measured



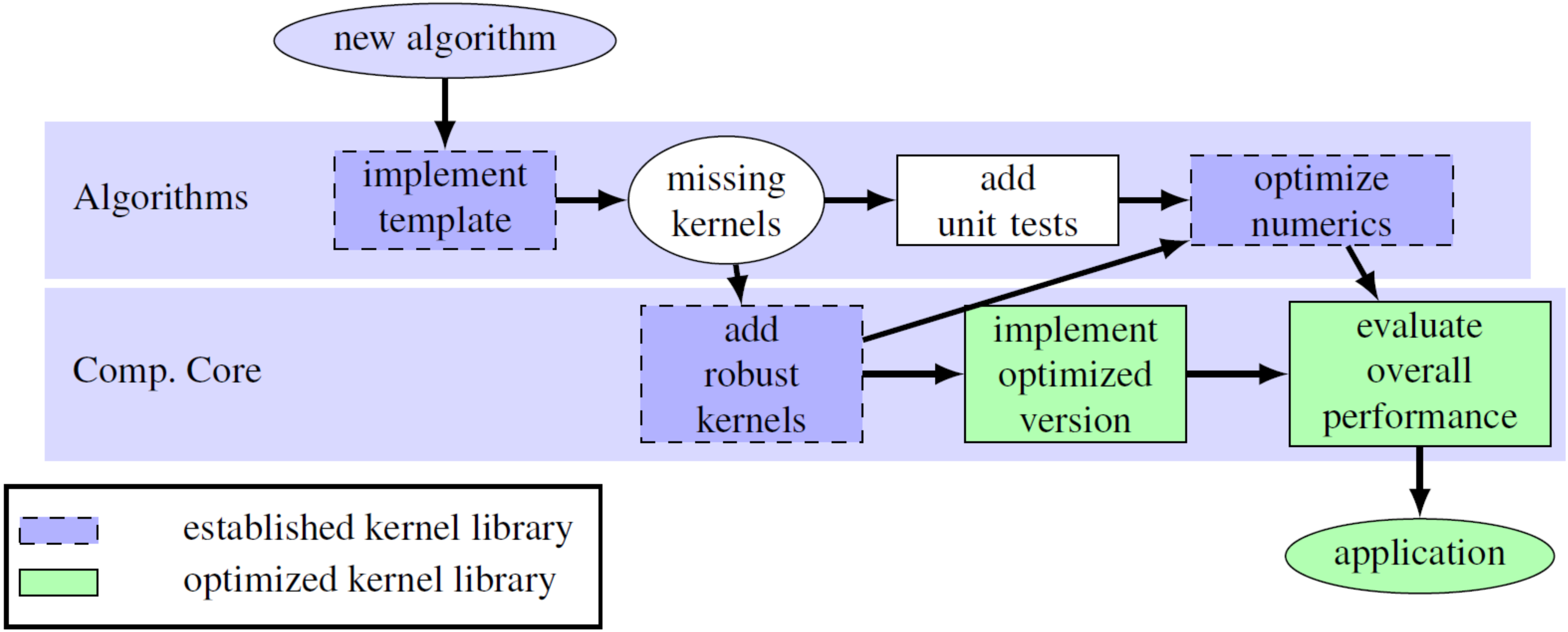
The ESSEX Software Infrastructure: PHIST for Implementing Iterative Solvers

a Pipelined Hybrid-parallel Iterative Solver Toolkit

- facilitate algorithm development using GHOST
- holistic performance engineering
- portability and interoperability



The ESSEX Software Infrastructure: Test-Driven Algorithm Development

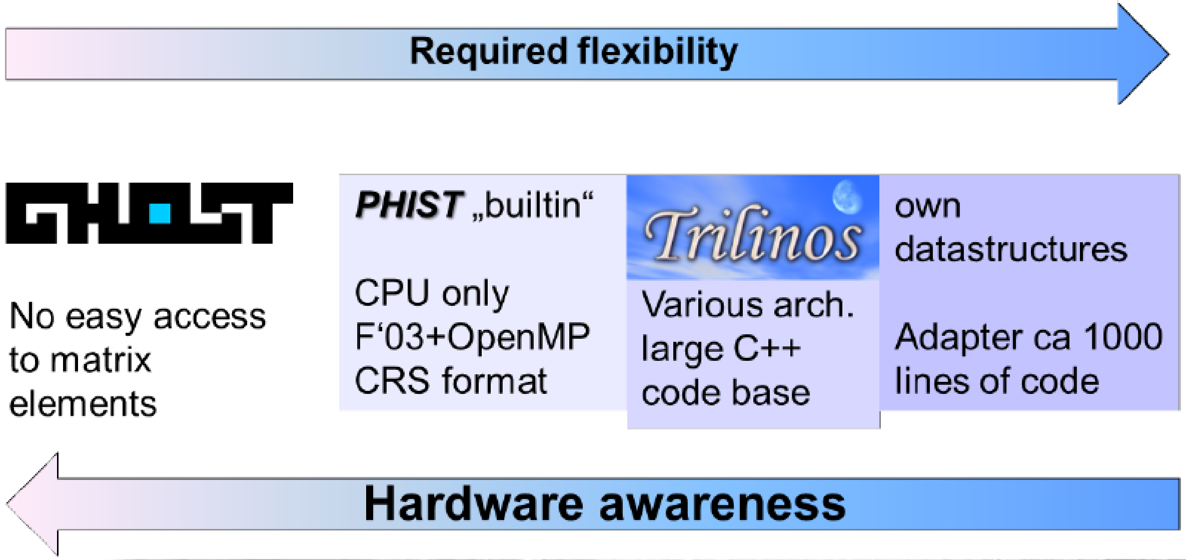


The ESSEX Software Infrastructure: PHIST for Implementing Iterative Solvers

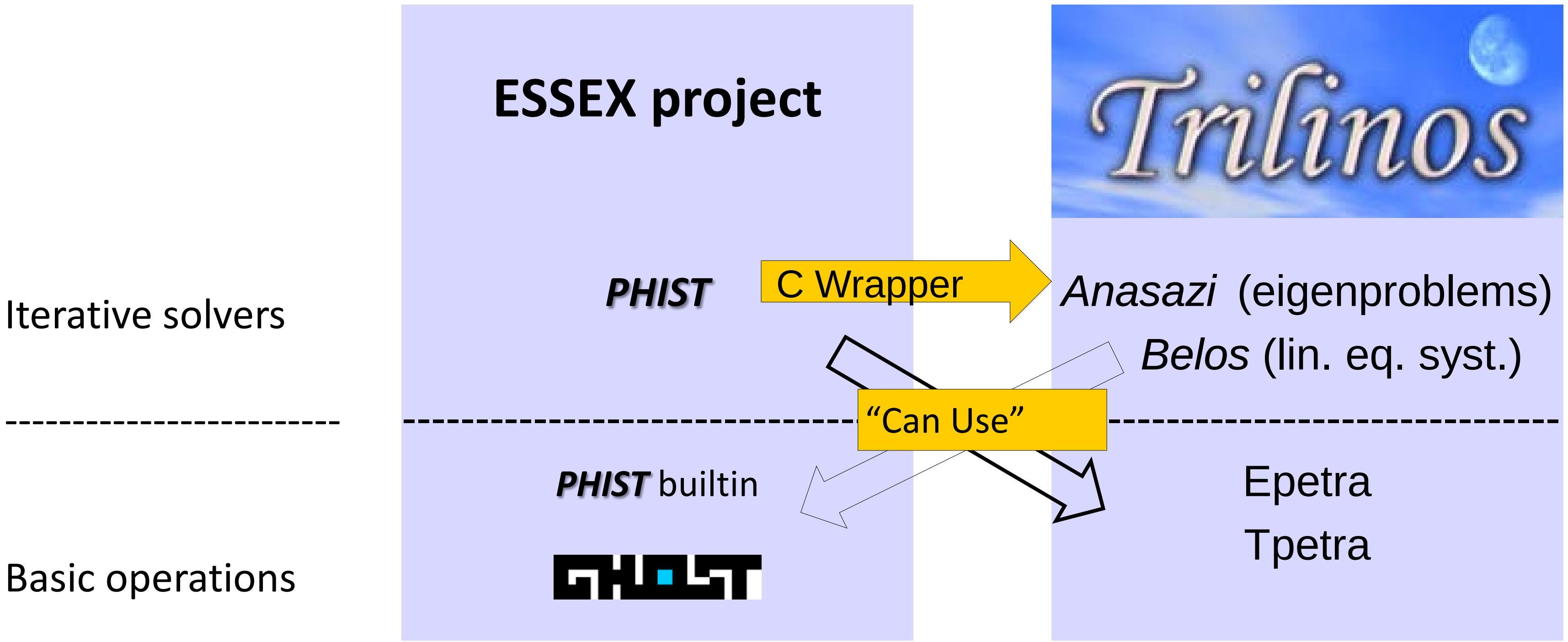
Useful abstraction: kernel interface

Choose from several 'backends' at compile time, to

- easily use **PHIST** in existing applications
- perform the same run with different kernel libraries
- compare numerical accuracy and performance
- exploit unique features of a kernel library (e.g. preconditioners)



Interoperability of PHIST and Trilinos



The ESSEX Software Infrastructure: PHIST for Implementing Iterative Solvers

Cool features of PHIST

Task macros

out-of-order execution of code blocks

- overlap comm. and comp.
- asynchronous checkpointing
- ...

Consistent random vectors

make **PHIST** runs comparable

- across platforms (CPU, GPU...)
- across kernel libraries
- independent of #procs, #threads

PerfCheck:

print achieved roofline performance of kernels after complete run to reveal

- deficiencies of kernel lib
- implementation issues of algorithm (strided data access etc.)

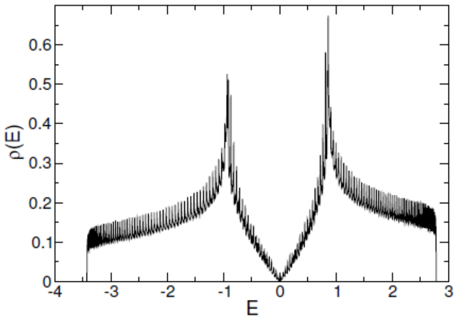
Special-purpose operations

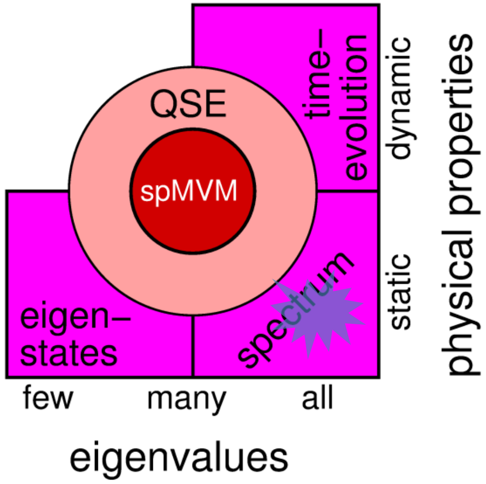
- fused kernels, e.g. compute $Y = \alpha AX + \beta Y$ *and* $Y^T X$
- highly accurate core functions, e.g. block orthogonalization in simulated quad precision

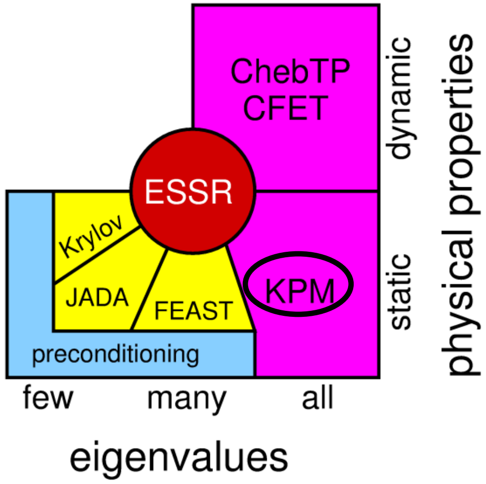
Application, Algorithm and Performance: Kernel Polynomial Method (KPM) – A Holistic View

- Compute **approximation to the complete eigenvalue spectrum** of large sparse matrix A (with $X = I$)

$$X(\omega) = \frac{1}{N}\mathrm{tr}[\delta(\omega - H)X] = \frac{1}{N}\sum_{n=1}^{N}\delta(\omega - E_n)\langle\psi_n, X\psi_n\rangle$$







The Kernel Polynomial Method (KPM)

Optimal performance exploit knowledge from all software layers!

Basic algorithm – Compute Cheyshev polynomials/moments:

for $r = 0$ to $R-1$ **do**
$\quad |v\rangle \leftarrow |\text{rand}()\rangle$
$\quad$ Initialization steps and computation of η_0, η_1
$\quad$ **for** $m = 1$ to $M/2$ **do**
$\quad\quad \text{swap}(|w\rangle, |v\rangle)$
$\quad\quad |u\rangle \leftarrow H|v\rangle$ ▷ spmv()
$\quad\quad |u\rangle \leftarrow |u\rangle - b|v\rangle$ ▷ axpy()
$\quad\quad |w\rangle \leftarrow -|w\rangle$ ▷ scal()
$\quad\quad |w\rangle \leftarrow |w\rangle + 2a|u\rangle$ ▷ axpy()
$\quad\quad \eta_{2m} \leftarrow \langle v|v\rangle$ ▷ nrm2()
$\quad\quad \eta_{2m+1} \leftarrow \langle w|v\rangle$ ▷ dot()
$\quad$ **end for**
end for

Application:
Loop over random initial states

Algorithm:
Loop over moments

Building blocks:
(Sparse) linear algebra library

- spmv() – Sparse matrix vector multiply
- axpy() – Scaled vector addition
- scal() – Vector scale
- axpy() – Scaled vector addition
- nrm2() – Vector norm
- dot() – Dot Product

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The Kernel Polynomial Method (KPM)

Optimal performance exploit knowledge from all software layers!

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for $r = 0$ to $R-1$ **do**
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    $\eta_{2m} \leftarrow \langle v|v\rangle$ ▷ nrm2()
    $\eta_{2m+1} \leftarrow \langle w|v\rangle$ ▷ dot()
  end for
end for

⇒

for $r = 0$ to $R-1$ **do**
  $|v\rangle \leftarrow |\text{rand}()\rangle$
  Initialization steps and computation of η_0, η_1
  for $m = 1$ to $M/2$ **do**
    swap($|w\rangle, |v\rangle$)
    $|w\rangle = 2a(H - b\mathbb{1})|v\rangle - |w\rangle$ &
      $\eta_{2m} = \langle v|v\rangle$ &
      $\eta_{2m+1} = \langle w|v\rangle$ ▷ aug_spmv()
  end for

Augmented Sparse Matrix Vector Multiply

The Kernel Polynomial Method (KPM)

Optimal performance exploit knowledge from all software layers!

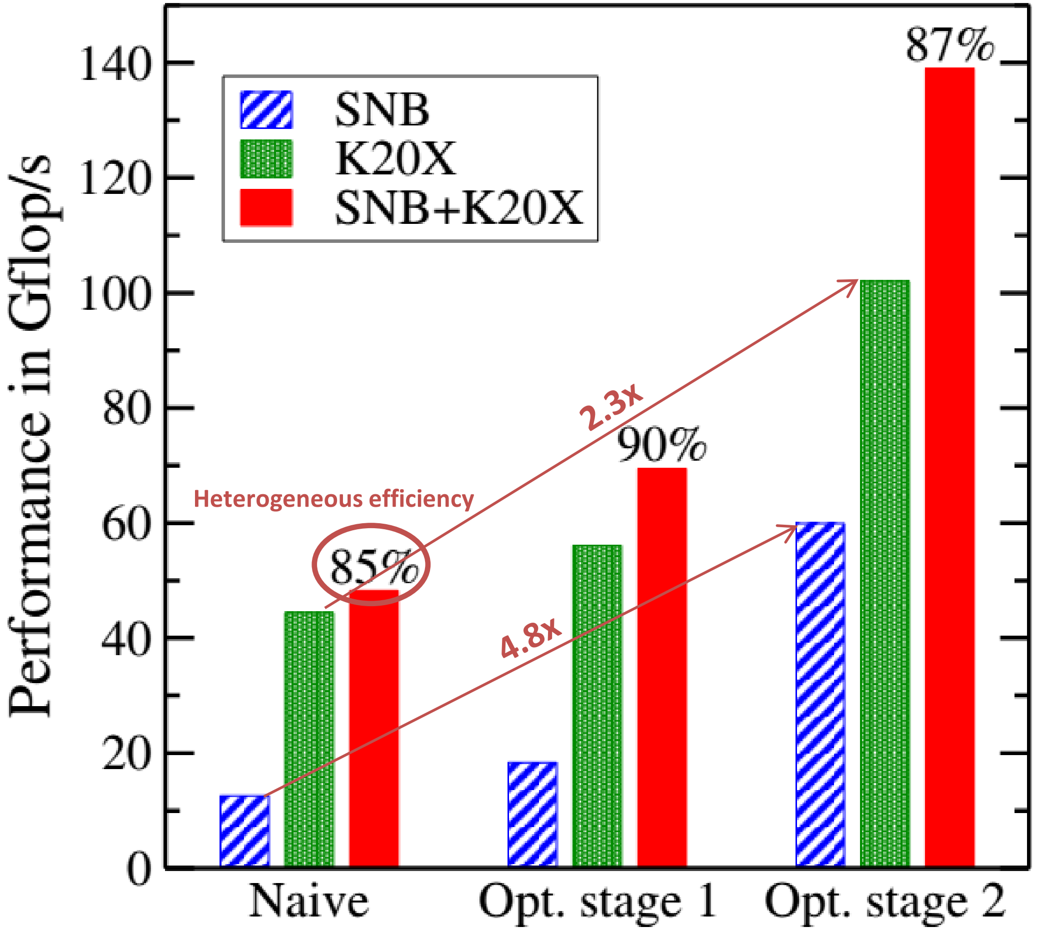
Basic algorithm – Compute Cheyshev polynomials/moments:

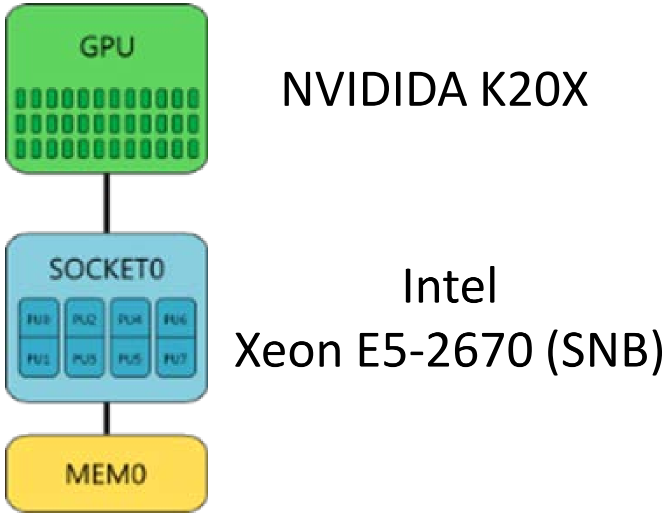
for $r = 0$ to $R-1$ **do**
  $|v\rangle \leftarrow |\text{rand}()\rangle$
  Initialization steps and computation of η_0, η_1
  for $m = 1$ to $M/2$ **do**
    $\text{swap}(|w\rangle, |v\rangle)$
    $|w\rangle = 2a(H - b\mathbb{1})|v\rangle - |w\rangle$ &
      $\eta_{2m} = \langle v|v\rangle$ &
      $\eta_{2m+1} = \langle w|v\rangle$ ▷ aug_spmv()
  end for

$|V\rangle := |v\rangle_{0..R-1}$ ▷ Assemble vector blocks
$|W\rangle := |w\rangle_{0..R-1}$
$|V\rangle \leftarrow |\text{rand}()\rangle$
Initialization steps and computation of μ_0, μ_1
for $m = 1$ to $M/2$ **do**
  $\text{swap}(|W\rangle, |V\rangle)$
  $|W\rangle = 2a(H - b\mathbb{1})|V\rangle - |W\rangle$ &
    $\eta_{2m}[:] = \langle V|V\rangle$ &
    $\eta_{2m+1}[:] = \langle W|V\rangle$ ▷ aug_spmmv()
end for

Augmented Sparse Matrix
Multiple Vector Multiply

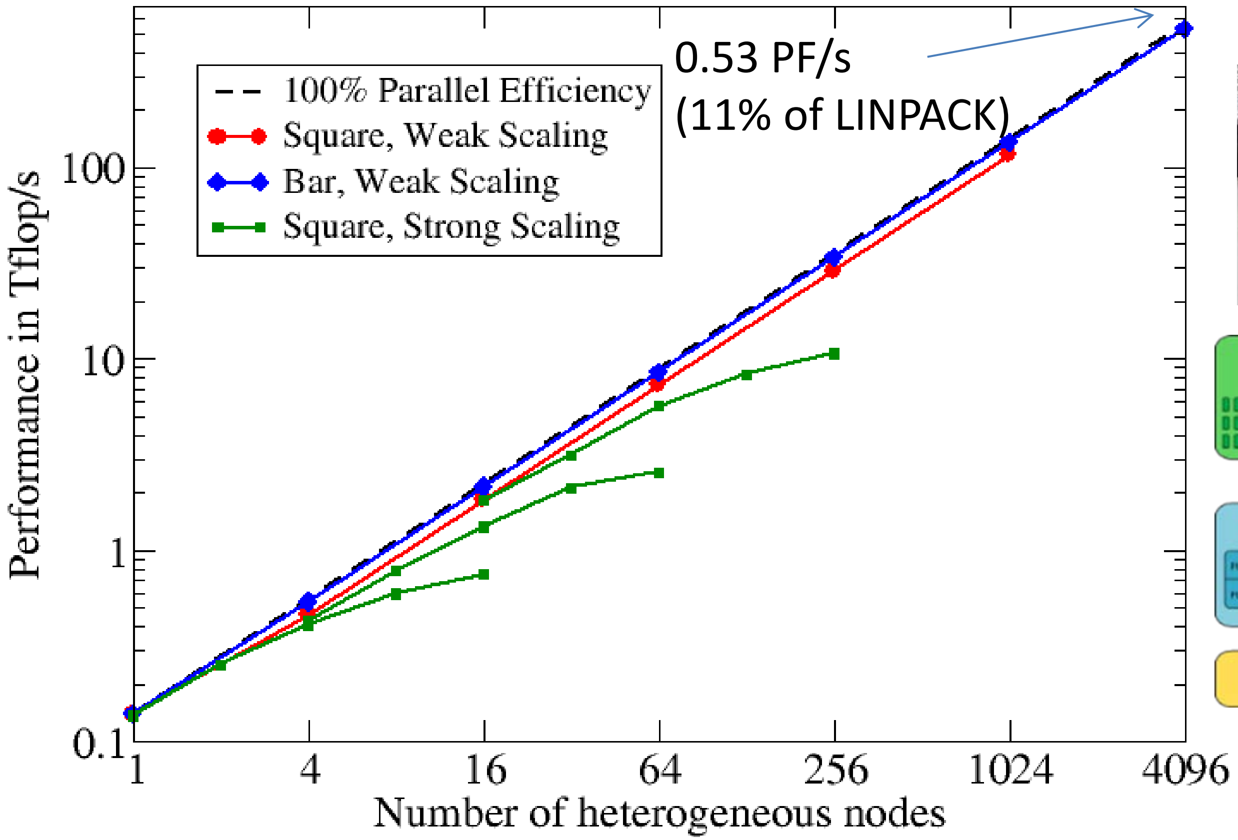
KPM: Heterogenous Node Performance



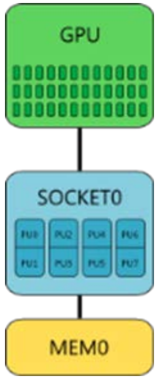


- Topological Insulator Application
- Double complex computations
- Data parallel static workload distribution

KPM: Large Scale Heterogenous Node Performance



CRAY XC30 – PizDaint*



- 5272 nodes
- Peak: 7.8 PF/s
- LINPACK: 6.3 PF/s
- Largest system in Europe

Performance Engineering of the Kernel Polynomial Method on Large-Scale CPU-GPU Systems
M. Kreutzer, A. Pieper, G. Hager, A. Alvermann, G. Wellein and H. Fehske, IEEE IPDPS 2015

*Thanks to CSCS/T. Schulthess for granting access and compute time

Conclusions

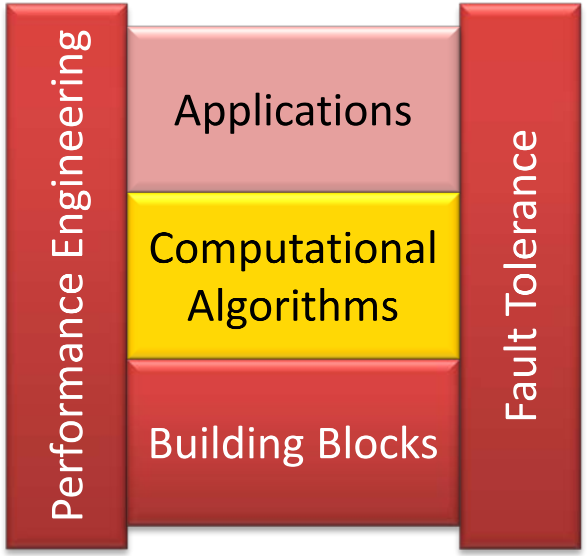
- Holistic performance engineering strategie successful for developing highly scalable solutions, cf. KPM.
- ***PHIST*** with GHOST provides a pragmatic, flexible and hardware-aware programming model for heterogeneous systems.
  - Includes highly scalable sparse iterative solvers for eigenproblems and systems of linear equations
  - Well suited for iterative solver development and solver integration into applications
- First convincing results with quantum physics applications

Future Work: Programming

Extended

Building Blocks, Parallelization, and Performance Engineering

- Holistic performance and power engineering
- Advanced building blocks engineering



Extended

Fault Tolerance

- From prototype to application software
  - Asynchronous checkpointing & I/O
  - Automatically fault-tolerant applications

NEW

Numerical Reliability

- Performance aspects
  - Silent data corruption / skeptical programming
  - High-precision reduction operations

Thanks

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Computer Science, Univ. Erlangen

Applied Computer Science, Univ. Wuppertal

Institute for Physics, Univ. Greifswald

Erlangen Regional Computing Center

- project website incl. list of publications: http://blogs.fau.de/essex/
- source code: https://bitbucket.org/essex/[ghost|phist]

International contacts

Sandia (Trilinos project)
Tenessee (Dongarra)
Japan: Tsukuba, Tokyo
The Netherlands: Groningen, Utrecht

Many thanks for your attention!

Questions?

Dr.-Ing. Achim Basermann

German Aerospace Center (DLR)

Simulation and Software Technology

Department High-Performance Computing

Achim.Basermann@dlr.de

http://www.DLR.de/sc