Algorithm and Library Software Design – Challenges for Tera, Peta, and Future Exascale Computing

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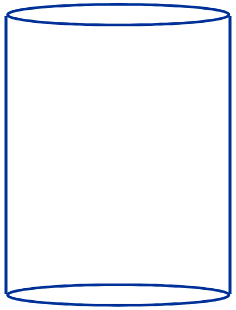
Outline

- Parallel computing
  - what, why and how?
- Parallel computer systems
  - today and the future
- European Exascale Software Initiative (ESSI)
- Algorithm and software design - critical issues
  - Aims: scalability, efficiency, portability, robustness

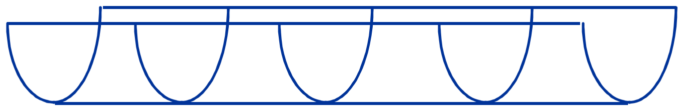
Can all problems be solved in parallel?

Dig a hole:



Can be done in parallel? Yes ☐ No ☐

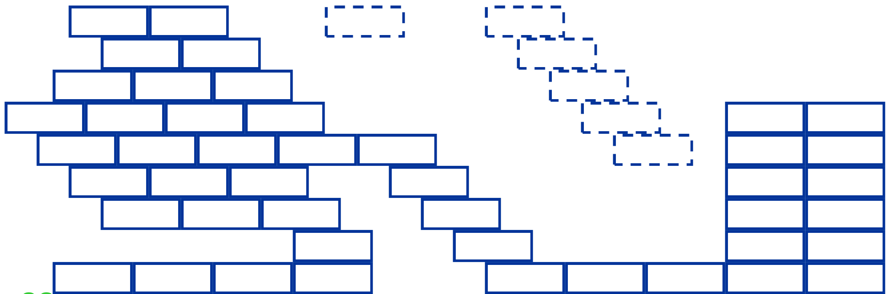
Dig a ditch:



Can be done in parallel? Yes ☐ No ☐

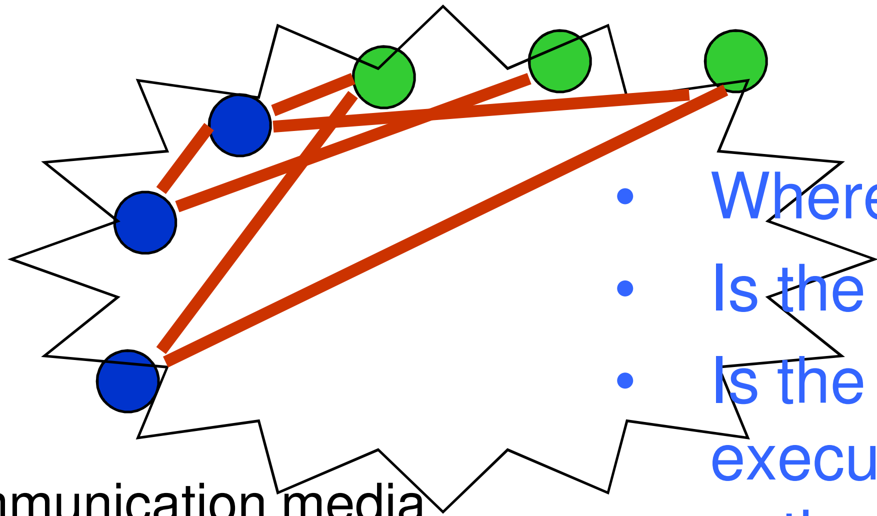
Brick a wall:

Can a stone be placed Anywhere at anytime? Yes ☐ No ☐



Parallel computing

A collection of processors (nodes) that communicate and cooperate to solve a large problem fast and reliably.



Communication media

- Where is the data placed?
- Is the workload balanced?
- Is the allocation and execution of work tasks optimal?

Parallel algorithm design

- Data locality
  Where is the data placed?
  Should be close to ”processor” that needs it!
- Load balance of computational work
  Is the workload balanced?
  All processors should do same amount of work!
- Schedule to minimize idle time
  Are the work tasks done in an optimal order?
  Remove redundant synchronization overhead!

In general, NP-complete!

Parallelism everywhere – new great challenges!

- Parallel architectures
  - From laptops to supercomputers
  - Paradigms: SM (e.g., multicore), DM, hybrid, graphics processing units (GPU)

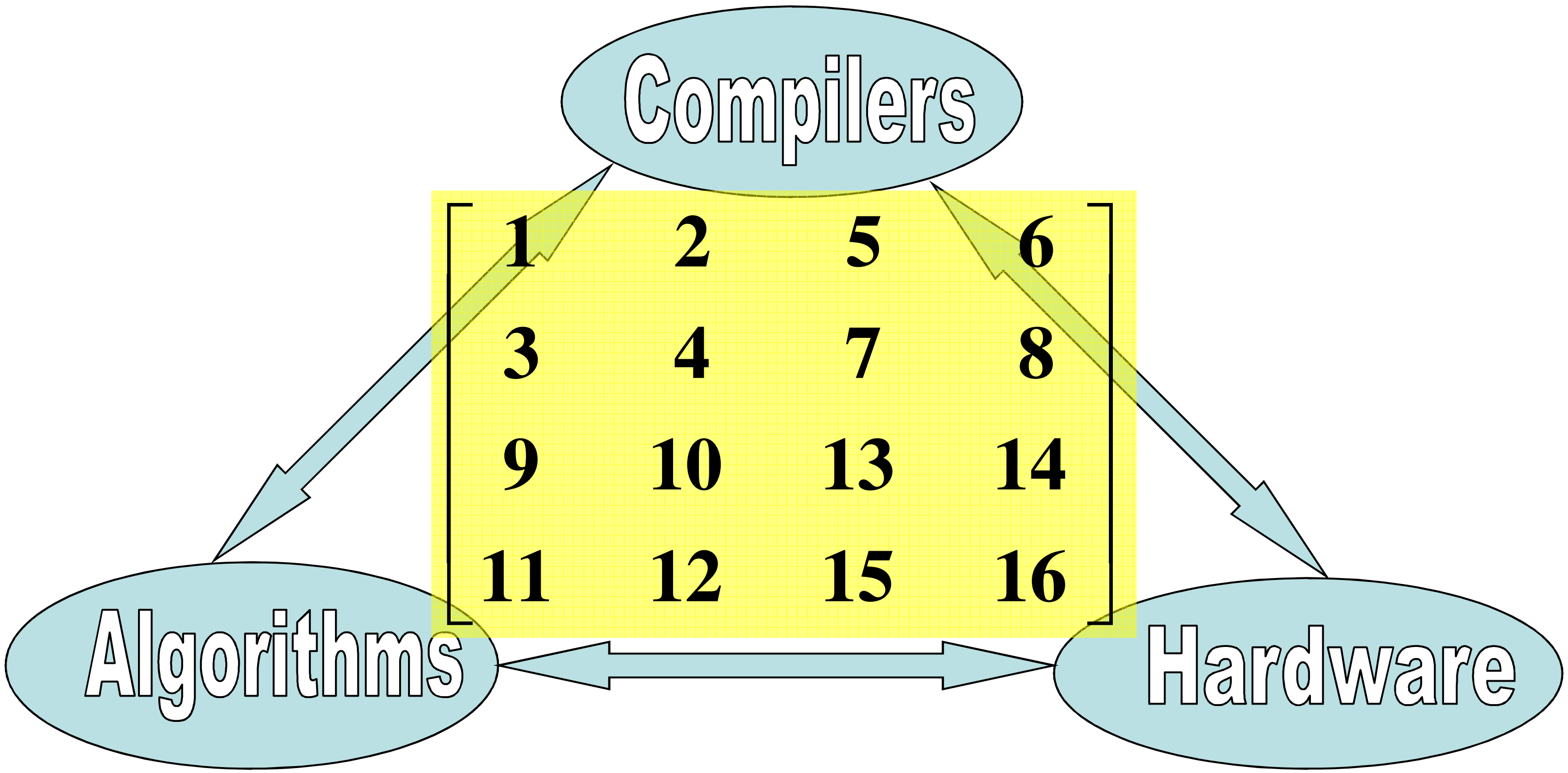
- Great increasing demand for *methods, tools, algorithms, languages and (library) software* which support massive parallelism effectively!

Applications demand unlimited amount of resources (flops, bytes):

Tera = 10^{12} → Peta = 10^{15} → Exa = 10^{18}

Key to performance?

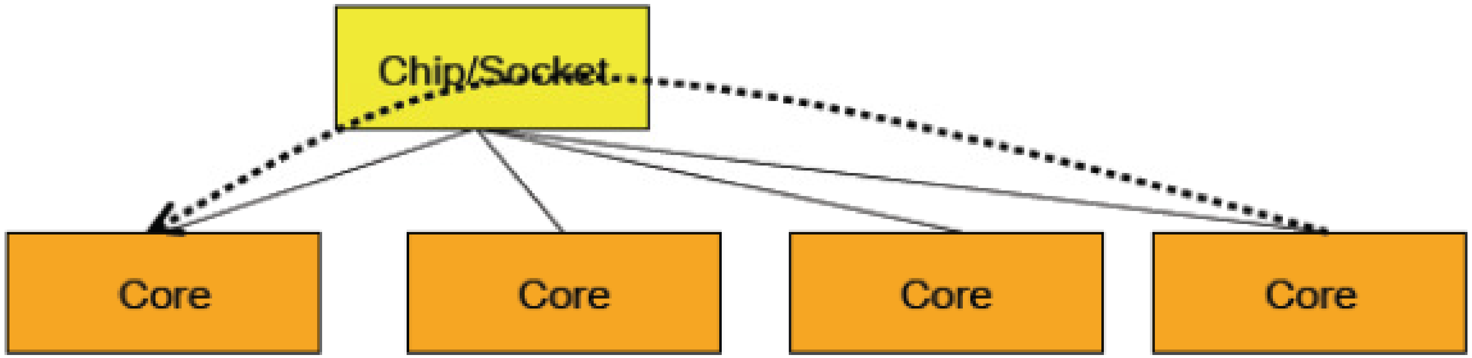
To understand the algorithm and architecture interaction!



Parallel system of today

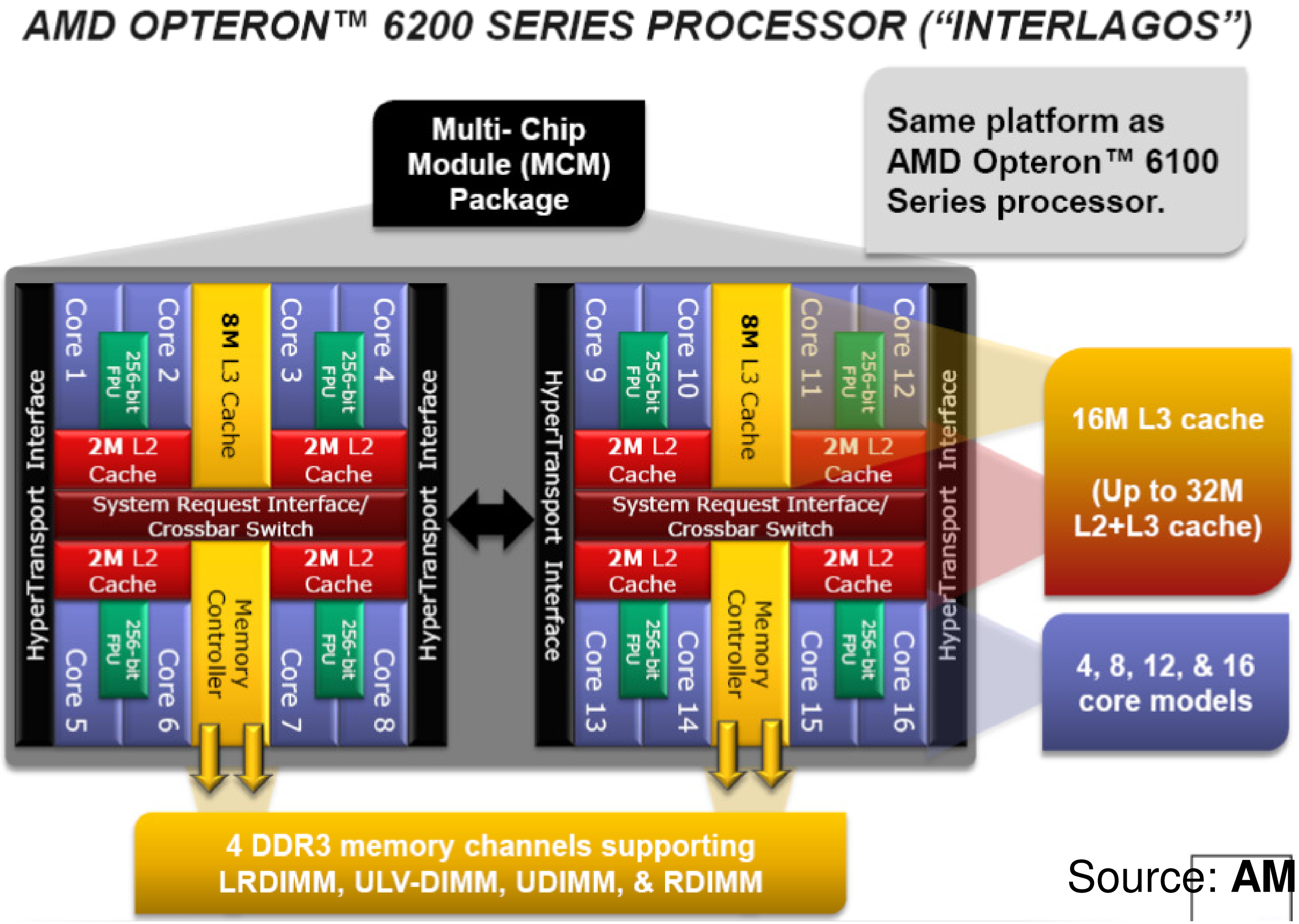
- Multi-level parallelism in architecture designs
- Multi-level memory hierarchies

Parallelism at processor level:



Source: **ICL at UT**

Parallel system of today

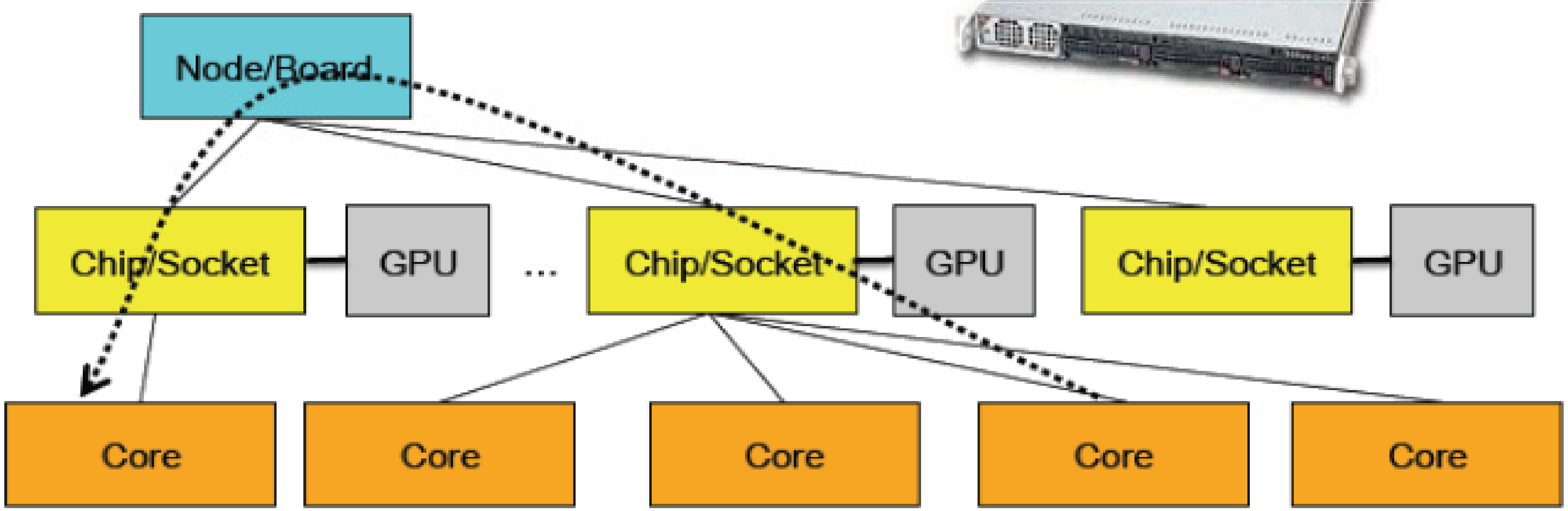


Source: **AMD**

Parallel system of today

Node Board:

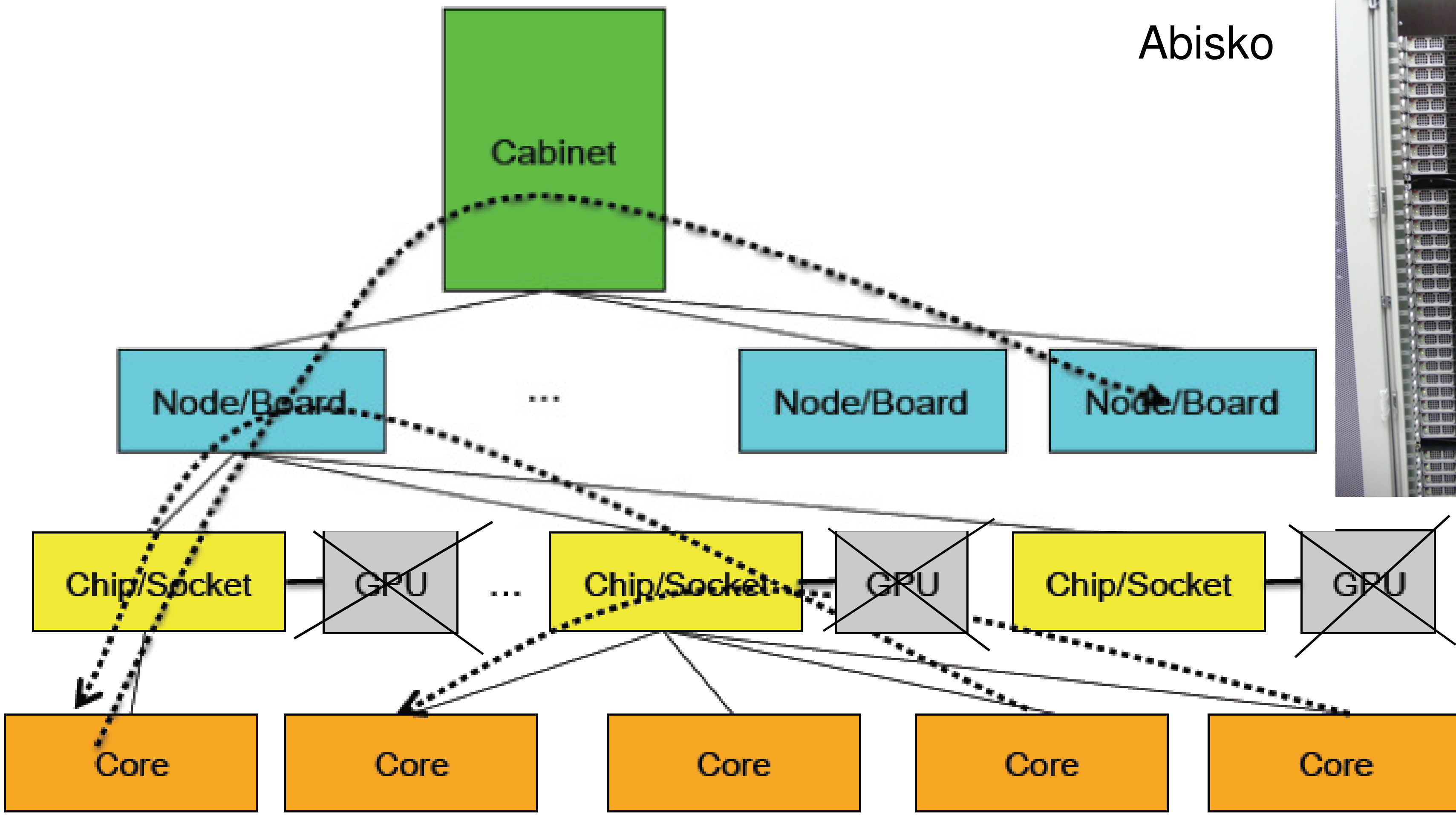
- Several chips/sockets per node
- Accelerators



Source: **ICL at UT**

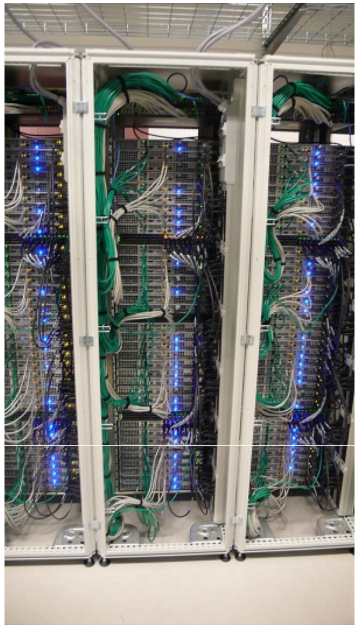
Parallel system of today

Abisko



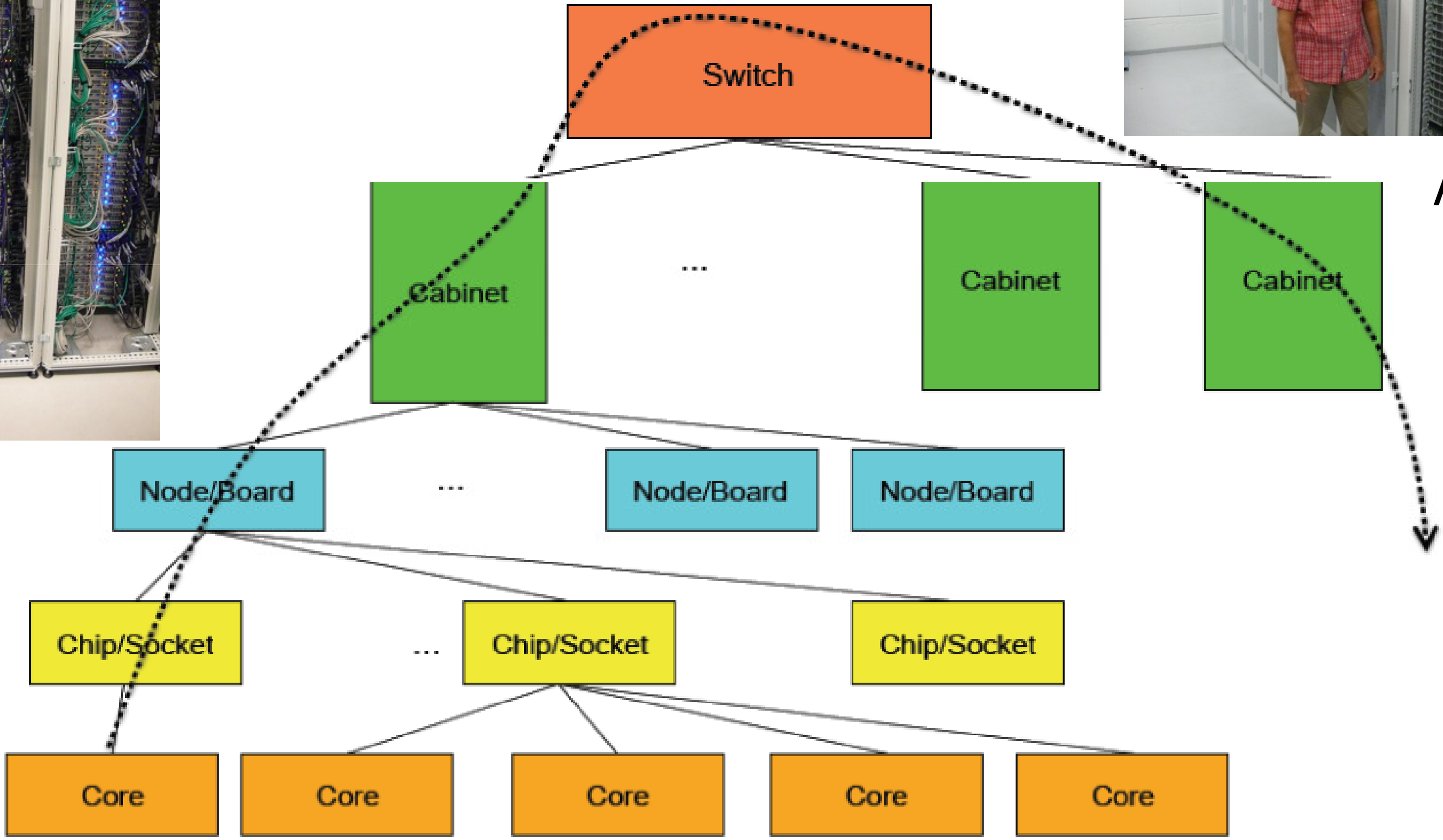
Source: **ICL at UT**

Parallel system of today



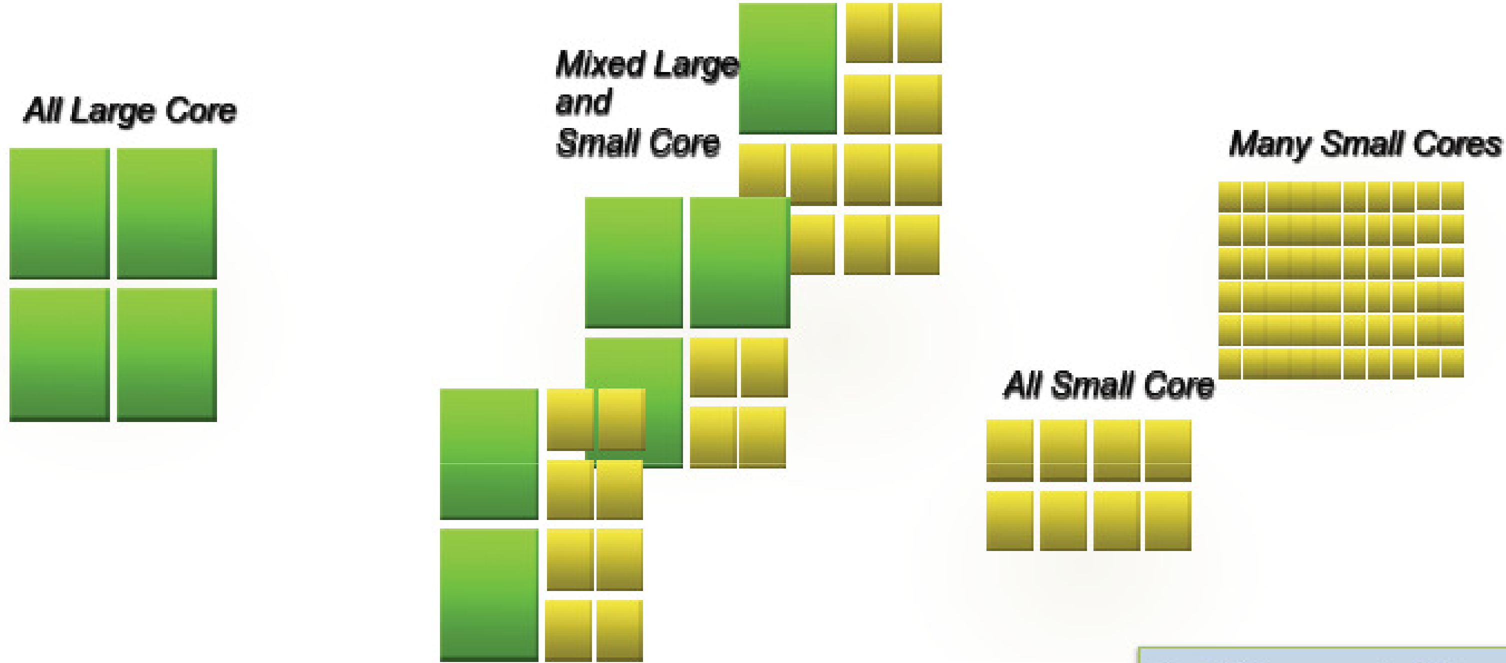
Combination of **shared memory** and **distributed memory programming**

Abisko

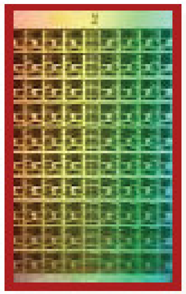


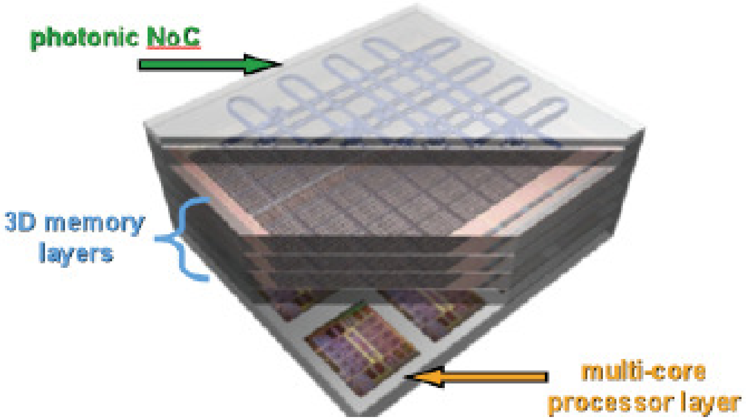
Source: **ICL at UT**

Future parallel systems?



Many Floating-Point Cores





Different Classes of Chips

- Home
- Games / Graphics
- Business
- Scientific

Source: **ICL at UT**

European Exascale Software Initiative

- **Objective:**
  To build a European vision and roadmap to address the challenges of the new generation of massively parallel systems composed of millions of heterogeneous cores which will provide multi-Petaflop performances in the next few years and Exaflop performances in 2020.
- Co-funded by the European Commission.

- **IESP -** International Exascale Software Project
  co-funded by DOE and NSF in USA.

EESI working groups

WP3: Application Grand Challenges	
WP Chair: Stéphane Requena (GENCI)	
	Chair
WG 3.1 Industrial and Engineering Applications	Philippe Ricoux (TOTAL)
WG 3.2 Weather, Climatology and Earth Sciences	Giovanni Aloisio (ENES-CMCC)
WG 3.3 Fundamental Sciences (Chemistry, Physics)	Godehard Sutmann (CECAM)
WG 3.4 Life Science and Health	Modesto Orozco (BSC)
WP4: Enabling Technologies for Exaflop Computing	
WP Chair: Bernd Mohr (Jülich)	
	Chair
WG 4.1 Hardware Roadmaps, Links with Vendors	Herbert Huber (STRATOS-LRZ)
WG 4.2 Software Eco-system	Franck Cappello (INRIA-UIUC)
WG 4.3 Numerical Libraries, Software and Algorithms	Iain Duff (STFC-RAL and CERFACS)
WG 4.4 Scientific Software Engineering	Mike Ashworth (STFC-DL)

WG 4.3 - Report

Numerical Libraries, Software and Algorithms:

- Dense linear algebra
- Graph and hypergraph partitioning
- Sparse direct methods
- Iterative methods for sparse matrices
- Eigenvalue problems, model reduction
- Optimization
- Control of complex systems
- Structured and unstructured grids

Much interdependence between areas.

Importance of also working at Tera- and Petascale levels!

Algorithm and software design – critical issues

- Reduce synchronization overhead
  - Dynamic scheduling and load balancing
- Hide and avoid communication and data movement
  - Blocking and remapping of data
- Use of mixed precision arithmetic
  - Refinement techniques
  - 2x speed of ops and 2x speed for data movement
- Reproducibility of results
  - Can not in general be guaranteed!
  - Error estimation of results

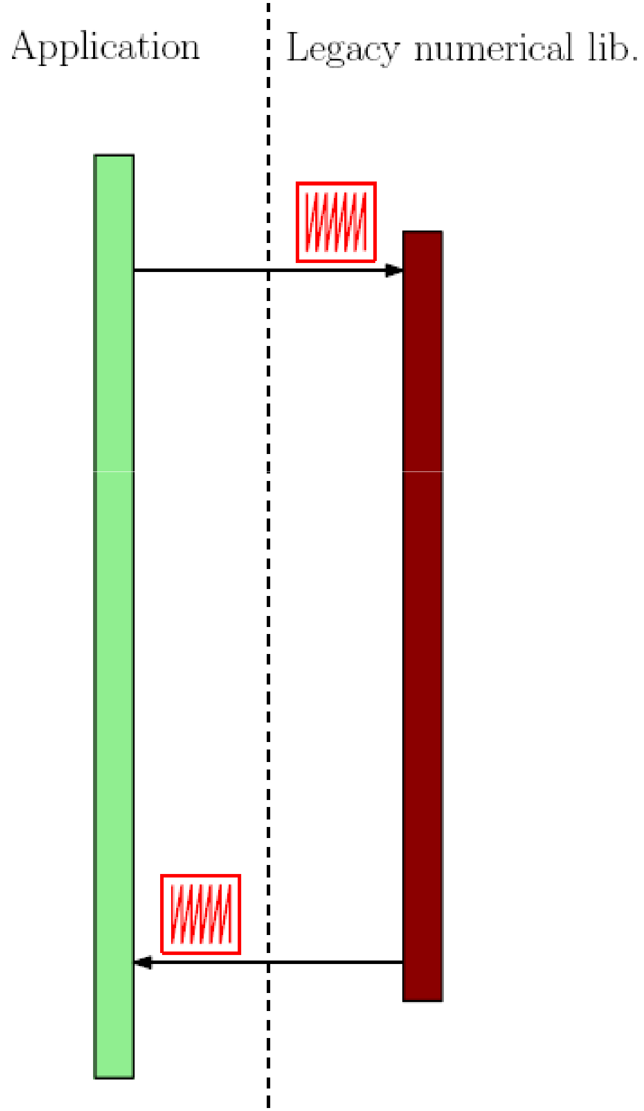
Algorithm and software design – critical issues

- Fault resilence (tolerance)
  - Recover from HW failures
  - Checkpointing, recomputation, redundant computation
  - Effect on accuracy and performance (speed) – a general trade-off issue!
- Autotuning and performance optimization
  - Build intelligence into software to adapt to hardware
- Energy aware algorithms
  - Frequence of cores can be controlled to save energy
  - Dynamic Voltage and Frequency Scaling (DVFS)

Application software using legacy HPC software

- Column-major (**CM**) and row-major (**RM**) storage formats are typically used by compilers
- BLAS, LAPACK, ScaLAPACK, etc. assume that inputs are in **CM** format

- Blocks are scattered in memory!
- Remedy: Use blocked data layouts internally!



Blocked storage formats

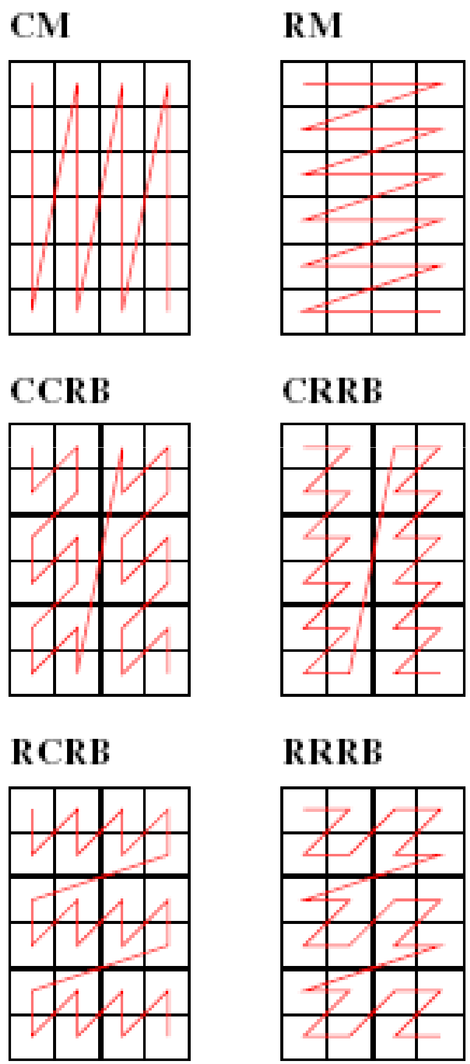
Standard formats

- **CM** Column-Major
- **RM** Row-Major
- Inefficient block access

Blocked formats

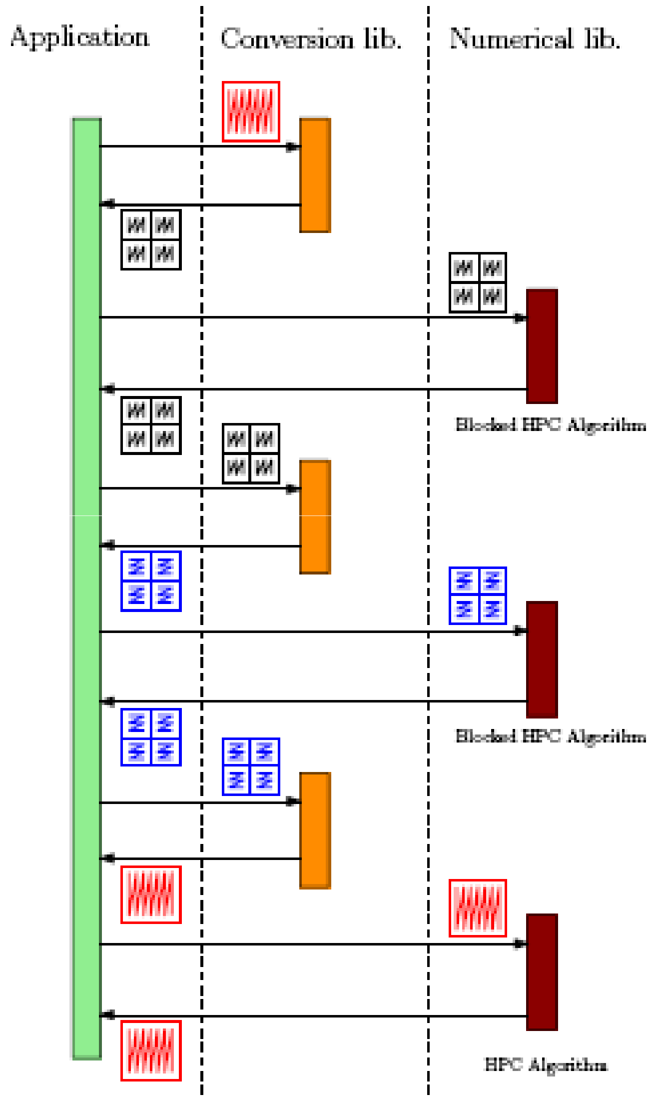
- **CCRB** Column-Column RB
- **CRRB** Column-Row RB
- **RCRB** Row-Column RB
- **RRRB** Row-Row RB
- Blocks are stored contiguously in memory

(RB = Rectangular Block)



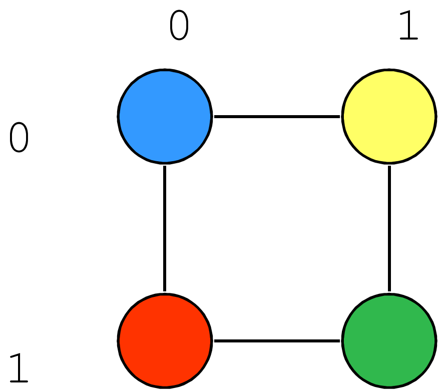
Application with mixed use of HPC library routines

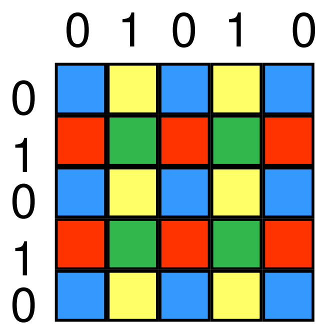
- CM → CCRB
- CCRB → RRRB
- RRRB → CM



Library design methodology

- Globally: explicit blocking and message passing for 2D block-cyclic data layouts

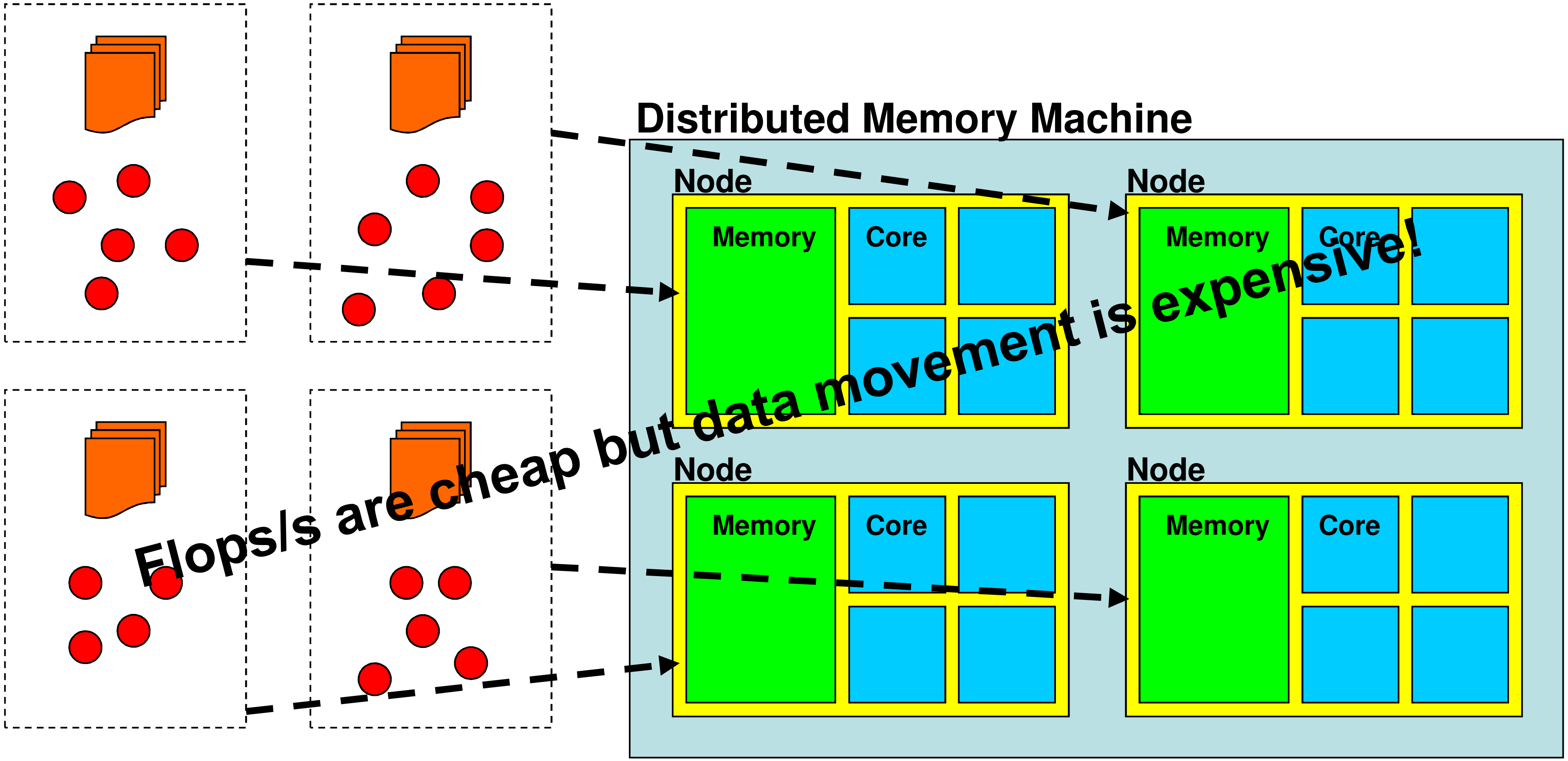




- Locally: explicit or recursive blocking and multi-threading for SMP/multicore nodes

Sample framework

- Global level: Static distribution of data and work
- Node level: Dynamic scheduling of work



Welcome to visit our poster!

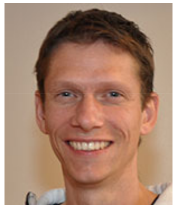
Efficient and Reliable HPC Algorithms for Matrix Computations in Applications

Sample projects

Björn Adlerborn, Andrii Dmytryshyn, Stefan Johansson, Lars Karlsson
Carl Christian Kjelgaard Mikkelsen, Bo Kågström (eSSENCE-PI), Meiyue Shao

Björn

Andrii



Stefan

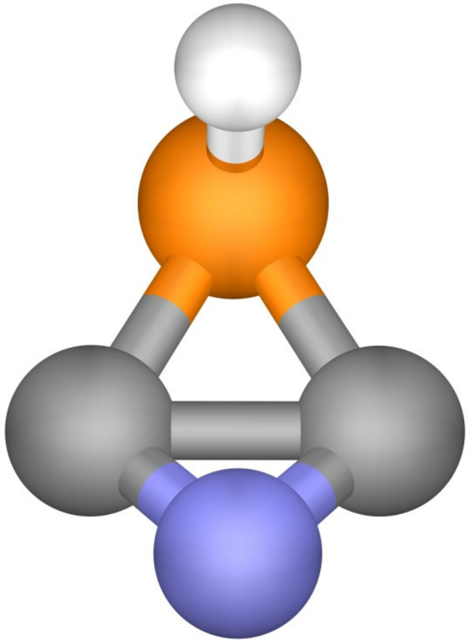
Lars

Carl Christian

Bo

Meiyue

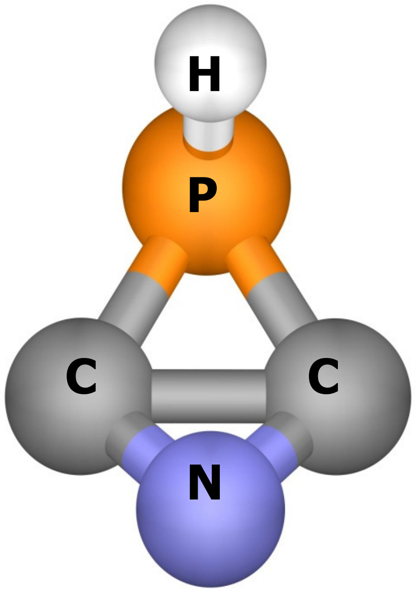
Thank you!



The HPC2N molecule

From macro- to micro- and further to nano-scale using Density Functional Theory!

”Nano-scale”



DFT computation, semi-stable, binding energy 15eV; Sven Öberg, LTU