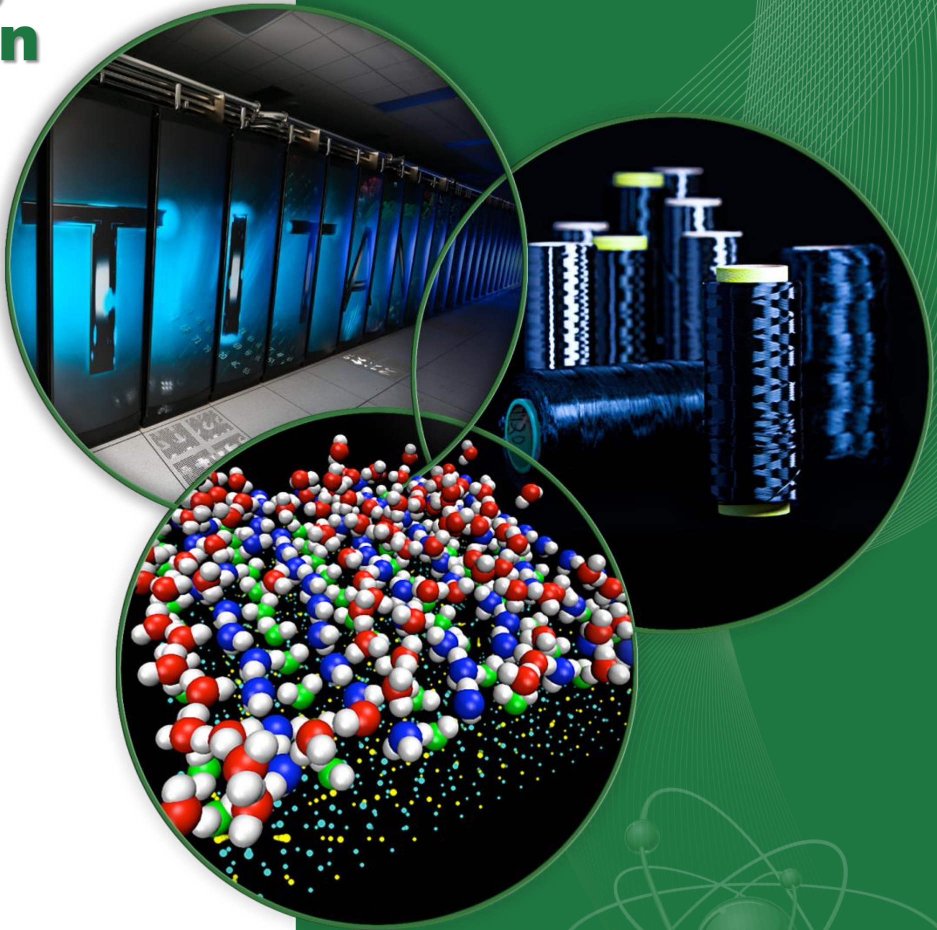
Dense/sparse numeric tensor algebra: Scalable, hardware-agnostic design for performance portability



Dmitry I. Lyakh

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Tensors

- Vector space ***A***:

$$\boldsymbol{A} \equiv span(\{a_i | i = 1 \dots m\})$$

- Vector space ***B***:

$$\boldsymbol{B} \equiv span(\{b_j | j = 1 \dots n\})$$

- Direct-product (tensor-product) space ***C***:

$$\boldsymbol{C} \equiv span\left(\left\{c_{ij} \equiv a_i b_j \middle| i = 1 \dots m, j = 1 \dots n\right\}\right)$$

- Dual basis:

$$a^i = g^{ij} a_j \qquad \overset{\text{Inner product}}{g_{ij} \equiv (a_i, a_j)} \qquad g^{ij} = (g_{ij})^{-1}$$

- Any vector space with a direct-product structure is represented by tensors

Applications

- Quantum many-body theory: Electronic and nuclear structure, quantum computing: Wave-function
- Loop quantum gravity: Fine structure of space-time
- Multivariate data analysis: Extracting correlations, features, data compression
- Classical physics
- Any data arranged as a multi-dimensional array is a tensor (in the most general sense)
- Any function of multiple variables discretized over a grid or some functional inner-product space is a tensor

CAAR Program @OLCF: Chemistry

- **DIRAC** (PI L. Visscher): Relativistic coupled-cluster theory
- **LS-DALTON** (PI P. Jorgensen): Local non-relativistic coupled-cluster theory for large molecular systems
- **NWChem** (PI K. Kowalski): Non-local non-relativistic coupled-cluster theory
- <u>Non-CAAR</u>: **ACES-IV** (PI R. Bartlett): Non-local non-relativistic coupled-cluster theory
- Other quantum-chemistry codes…

MATH: DENSE/BLOCK-SPARSE TENSOR ALGEBRA

Coupled-Cluster Theory

$$|\Psi\rangle = \exp(\hat{T})|0\rangle = \left(1 + \hat{T} + \frac{1}{2!}\hat{T}^2 + \frac{1}{3!}\hat{T}^3 + \frac{1}{4!}\hat{T}^4 + \cdots\right)|0\rangle$$

$$|\Psi_{excited}\rangle = \hat{R}e^{\hat{T}}|0\rangle$$

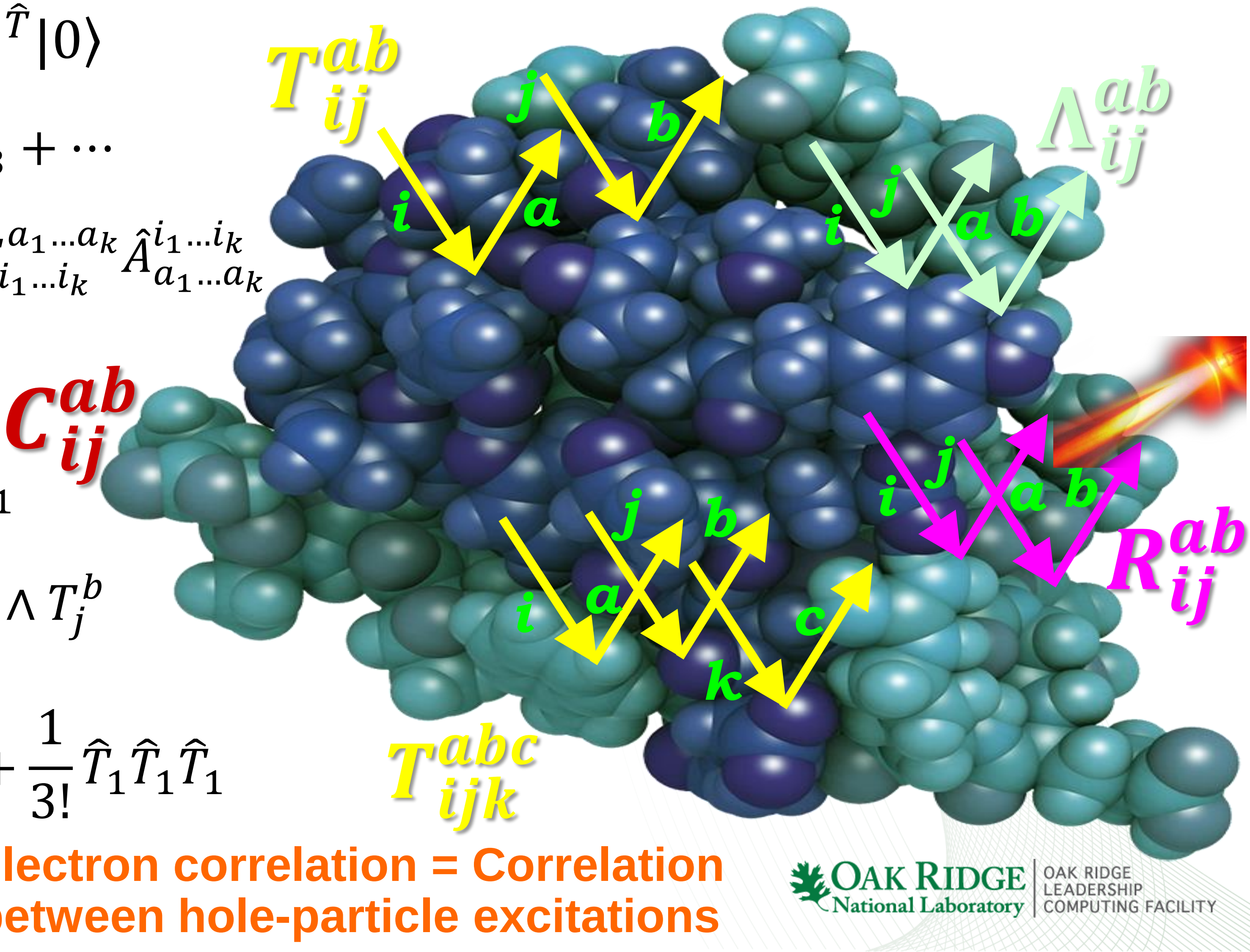
$$\hat{T} = \hat{T}_1 + \hat{T}_2 + \hat{T}_3 + \cdots$$

$$\hat{T}_k = \frac{1}{k!\,k!}\sum_{\substack{a_1\ldots a_k\\ i_1\ldots i_k}} T^{a_1\ldots a_k}_{i_1\ldots i_k}\hat{A}^{i_1\ldots i_k}_{a_1\ldots a_k}$$

$$\hat{C}_2 = \hat{T}_2 + \frac{1}{2!}\hat{T}_1\hat{T}_1$$

$$C^{ab}_{ij} = T^{ab}_{ij} + T^a_i \wedge T^b_j$$

$$\hat{C}_3 = \hat{T}_3 + \hat{T}_2\hat{T}_1 + \frac{1}{3!}\hat{T}_1\hat{T}_1\hat{T}_1$$



Electron correlation = Correlation between hole-particle excitations

Math Framework: Basic Tensor Algebra

- Formal tensor: $T^{pq...}_{rs...} \mapsto T(p,q,r,s,...)$: n-D Array

  Full tensor: $T(p,q,r,s): \; p \in P, q \in Q, r \in R, s \in S$

  Tensor slice: $T(p,q,r,s): \; p \in P' \subseteq P, q \in Q' \subseteq Q,$

  $r \in R' \subseteq R, s \in S' \subseteq S$

Few primitive operations:

- Tensor addition:

$$\forall p,q,r,s: \;\; T^{pq}_{rs} = L^{pq}_{rs} + R^{pq}_{rs}$$

Parallelism!

- Tensor product:

$$\forall p,q,r,s: \;\; T^{pq}_{rs} = L^{p}_{r} R^{q}_{s}$$

Parallelism!

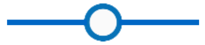
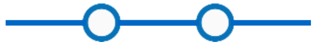
- Tensor contraction:

$$\forall p,q,r,s: \;\; T^{pq}_{rs} = L^{pai}_{bcd} R^{qbcd}_{rsai}$$

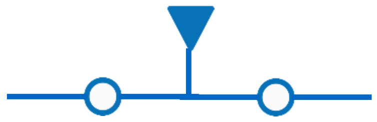
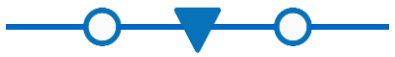
Compute intensive (potentially)!

Math Framework: Tensor Decompositions

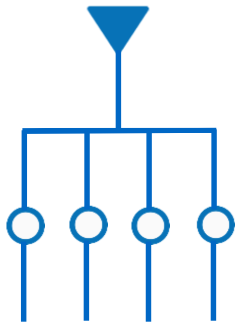
- Graphical (diagrammatic) representation:

Matrix:  Matrix*Matrix: 

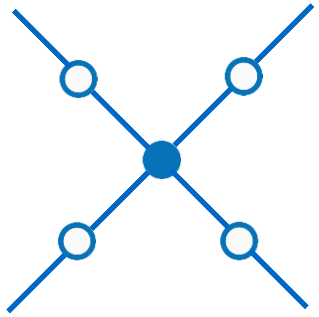
- Linear algebra: SVD is optimal in the 2-norm:

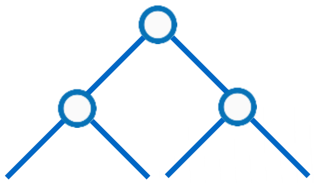
- Tensor (multi-linear) algebra: Many choices:



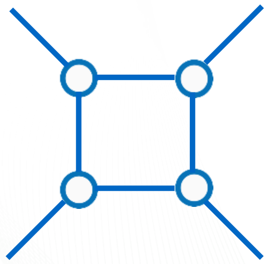
Canonical polyadic



Tucker



Tensor tree



Tensor train

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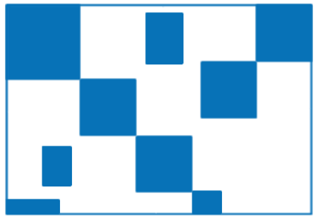
Tensor Sparsity

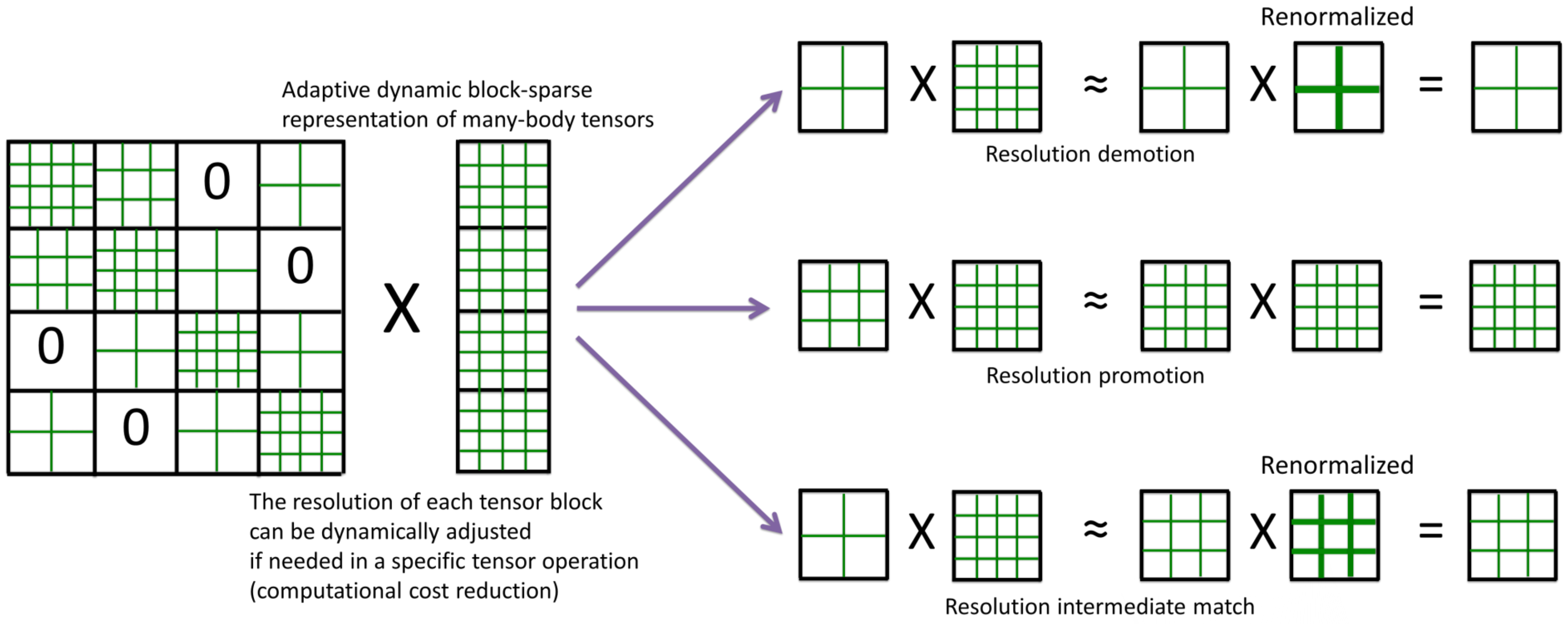
- Dense tensors:

- Block-sparse tensors:

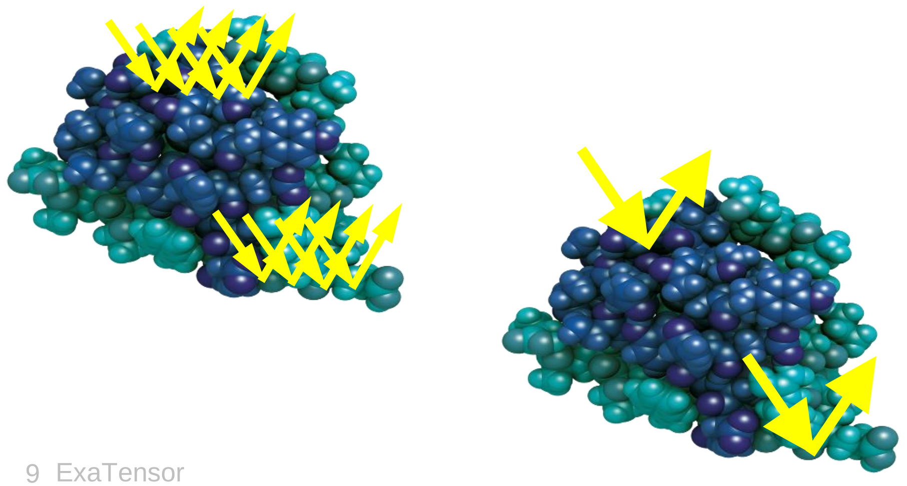


- Regular sparse tensors:
  - Some regular sparsity pattern other than block sparsity
- Irregular sparse tensors:
  - Sparsity pattern has no regularity

Resolution-Adaptive Tensor Algebra


Adaptive dynamic block-sparse representation of many-body tensors
0
0
0
0
X
Renormalized
X
≈
X
=
Resolution demotion
X
≈
X
=
Resolution promotion
Renormalized
X
≈
X
=
Resolution intermediate match

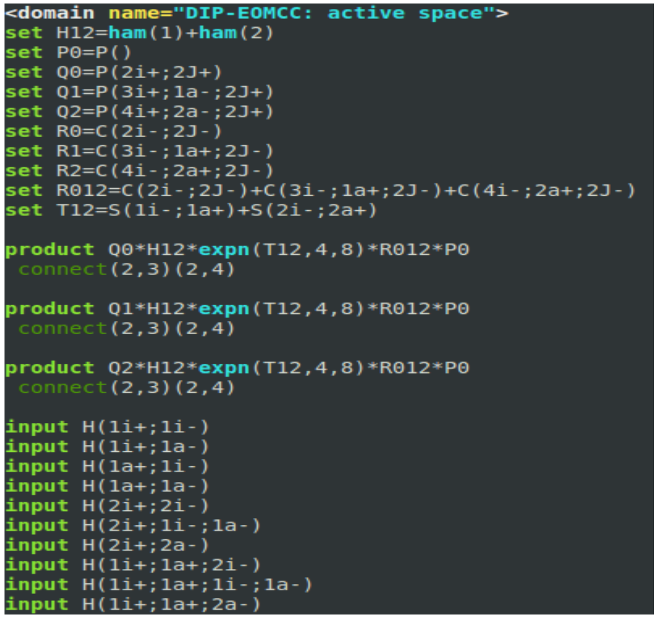
The resolution of each tensor block can be dynamically adjusted if needed in a specific tensor operation (computational cost reduction)



- Large tensor elements can become tensors themselves (higher resolution);
- Weak tensor slices can be compressed by lowering the resolution, up to a single (complex) number;
- Adapt to the calculated electronic state and available HPC resources;
- Should be better than just black-and-white discarding.

Automated Development Tools and DSL

- Automated equation/code generators are unavoidable in CC
- DSLangs and DSLibs can provide a scalable development environment: **DiaGen** input/output:



```
<domain name="DIP-EOMCC: active space">
set H12=ham(1)+ham(2)
set P0=P()
set Q0=P(2i+;2J+)
set Q1=P(3i+;1a-;2J+)
set Q2=P(4i+;2a-;2J+)
set R0=C(2i-;2J-)
set R1=C(3i-;1a+;2J-)
set R2=C(4i-;2a+;2J-)
set R012=C(2i-;2J-)+C(3i-;1a+;2J-)+C(4i-;2a+;2J-)
set T12=S(1i-;1a+)+S(2i-;2a+)

product Q0*H12*expn(T12,4,8)*R012*P0
 connect(2,3)(2,4)

product Q1*H12*expn(T12,4,8)*R012*P0
 connect(2,3)(2,4)

product Q2*H12*expn(T12,4,8)*R012*P0
 connect(2,3)(2,4)

input H(1i+;1i-)
input H(1i+;1a-)
input H(1a+;1i-)
input H(1a+;1a-)
input H(2i+;2i-)
input H(2i+;1i-;1a-)
input H(2i+;2a-)
input H(1i+;1a+;2i-)
input H(1i+;1a+;1i-;1a-)
input H(1i+;1a+;2a-)
```

(285) $192.3.896 : Z^{A^b_1}_{I^a_1 I^a_2 I^b_1} += H^{l^a_1 K^a_1}_{d^a_1, d^a_2} S^{d^a_1}_{I^a_1} S^{d^a_2}_{I^a_2} C^{A^b_1}_{I^b_1, l^a_1 K^a_1} \cdot +1/2$

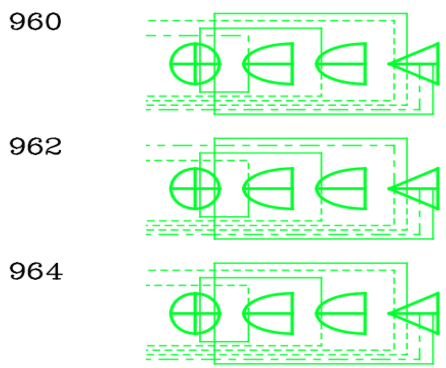
(286) $198.1.932 : Z^{A^b_1}_{I^a_1 I^a_2 I^b_1} += H^{l^b_1, l^b_2}_{d^b_1, d^b_2} S^{d^b_1}_{I^b_1} S^{d^b_2}_{l^b_1} C^{A^b_1}_{I^a_1 I^a_2, l^b_2}$

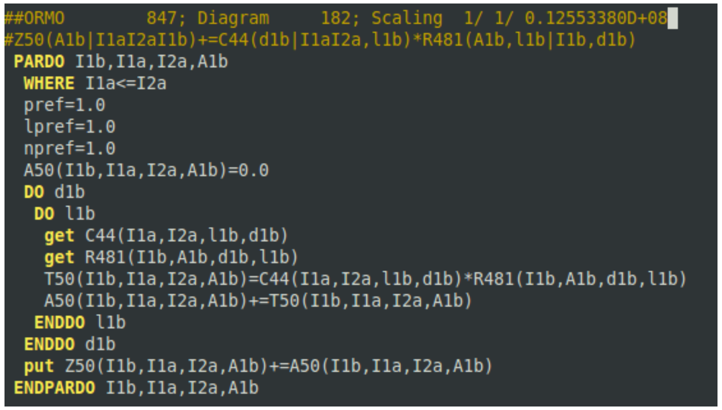
(287) $198.2.933 : Z^{A^b_1}_{I^a_1 I^a_2 I^b_1} += H^{l^b_1, l^a_1}_{d^a_1, d^b_1} S^{d^a_1}_{I^a_1} S^{d^b_1}_{l^b_1} C^{A^b_1}_{I^a_2 I^b_1, l^a_1}$

(288) $198.4.935 : Z^{A^b_1}_{I^a_1 I^a_2 I^b_1} += H^{l^a_1, l^b_1}_{d^b_1, d^a_1} S^{d^b_1}_{I^b_1} S^{d^a_1}_{l^a_1} C^{A^b_1}_{I^a_1 I^a_2, l^b_1}$

(289) $198.5.936 : Z^{A^b_1}_{I^a_1 I^a_2 I^b_1} += H^{l^a_1, l^a_2}_{d^a_1, d^a_2} S^{d^a_1}_{I^a_1} S^{d^a_2}_{l^a_1} C^{A^b_1}_{I^a_2 I^b_1, l^a_2}$

(290) $202.1.946 : Z^{A^b_1}_{I^a_1 I^a_2 I^b_1} += H^{l^b_1, K^a_1}_{d^a_1 d^b_1} S^{A^b_1}_{l^b_1} S^{d^a_1 d^b_1}_{I^a_1 I^b_1} C_{I^a_2, K^a_1}$





```
##ORMO        847; Diagram     182; Scaling  1/ 1/ 0.12553380D+08
#Z50(A1b|I1aI2aI1b)+=C44(d1b|I1aI2a,l1b)*R481(A1b,l1b|I1b,d1b)
 PARDO I1b,I1a,I2a,A1b
  WHERE I1a<=I2a
  pref=1.0
  lpref=1.0
  npref=1.0
  A50(I1b,I1a,I2a,A1b)=0.0
  DO d1b
   DO l1b
    get C44(I1a,I2a,l1b,d1b)
    get R481(I1b,A1b,d1b,l1b)
    T50(I1b,I1a,I2a,A1b)=C44(I1a,I2a,l1b,d1b)*R481(I1b,A1b,d1b,l1b)
    A50(I1b,I1a,I2a,A1b)+=T50(I1b,I1a,I2a,A1b)
   ENDDO l1b
  ENDDO d1b
  put Z50(I1b,I1a,I2a,A1b)+=A50(I1b,I1a,I2a,A1b)
 ENDPARDO I1b,I1a,I2a,A1b
```

(447) $324.85.1.1.3.1.0.20333376.09 : Z^{l^b_1}_{I^a_1 I^a_2 i^b_1} += H^{l^b_1, l^b_2}_{i^b_1, d^b_1} C^{d^b_1}_{I^a_1 I^a_2, l^b_2} \cdot -1.$

(448) $331.86.1.1.2.1.0.10042704.09 : Z^{l^b_1}_{I^a_1 I^a_2 i^b_1} += H^{l^b_1, K^a_1}_{I^a_1, d^b_1} C^{d^b_1}_{I^a_2 i^b_1, K^a_1} \cdot -1.$

(449) $325.85.1.1.3.1.0.20333376.09 : Z^{l^b_1}_{I^a_1 I^a_2 i^b_1} += H^{l^b_1, l^a_1}_{i^b_1, d^a_1} C^{d^a_1}_{I^a_1 I^a_2, l^a_1} \cdot -1.$

(450) $821.177.2.1.2.1.0.49593600.07 : Z^{l^b_1}_{I^a_1 I^a_2 i^b_1} += S^{d^b_1}_{i^b_1} R^{l^b_1}_{I^a_1 I^a_2, d^b_1} \cdot -1.$

(451) $938.199.1.2.2.2.0.11716488.10 : R^{l^b_1, K^a_1}_{I^a_1 i^b_1} += H^{l^b_1, K^a_1}_{d^a_1 d^b_1} S^{d^a_1 d^b_1}_{I^a_1 i^b_1}$

Efficient flexible runtime?

Computational Challenges

- Dense tensor algebra:
  - Communication bandwidth: Communication avoiding and regularization (similar to the matrix multiplication)
  - Memory size: Out-of-core algorithms
- Block-sparse tensor algebra:
  - Irregular data and workload: Load balancing → task-based programming model
- Resolution-adaptive block-sparse tensor algebra:
  - Dynamic irregular data and workload: Load balancing, dynamic data redistribution

Performance Portability Strategy

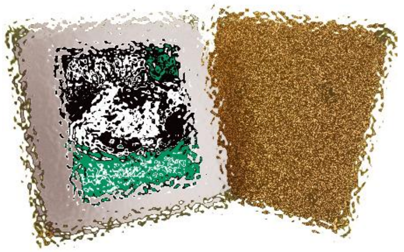
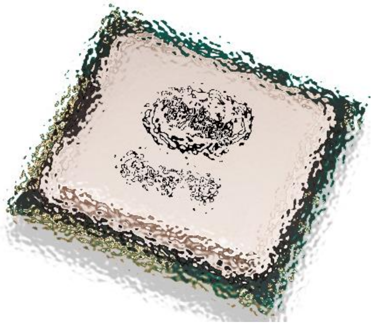
- **Abstract computing system**:
  - Distributed (weakly-coupled) level: The computing system is composed of compute nodes interconnected via network interfaces in accordance with some topology
  - (Semi-)shared (strongly-coupled) level: Each node is composed of multiple compute devices of the same or different kinds, possibly sharing the same (multi-level) memory
- Algorithms are formulated for this abstract computer
- The hardware specificity is masked by driver libraries that provide a device-unified API interface for a set of necessary domain-specific primitives
- New hardware = New driver library, done!

Node-Level Virtualization: Hiding Hardware

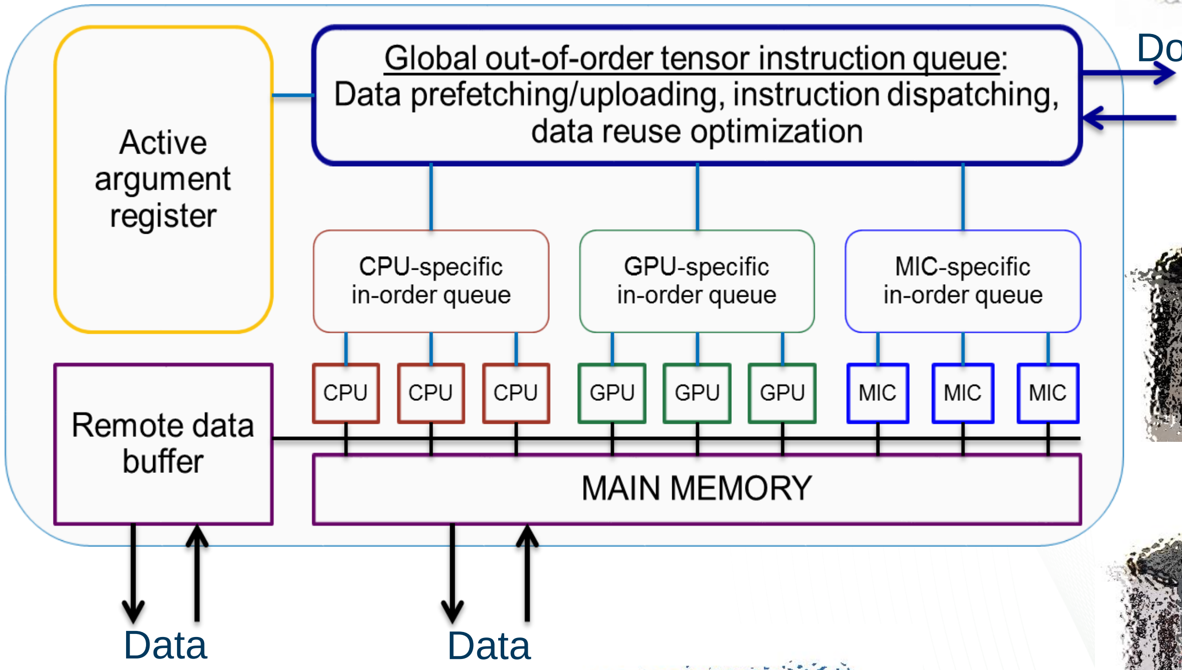
Hardware Processors (CPU, GPU, etc.)

Node-Level Virtualization: Hiding Hardware

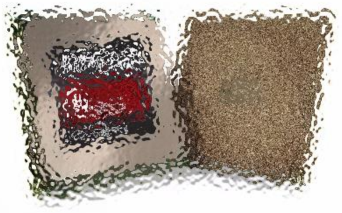
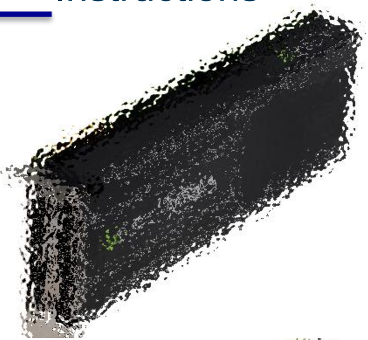
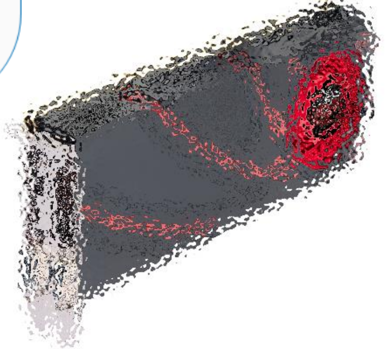
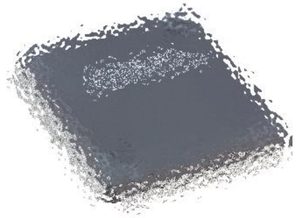
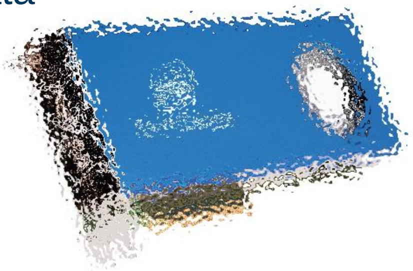
Domain-Specific Virtual Processor

ExaTensor Virtual Processor

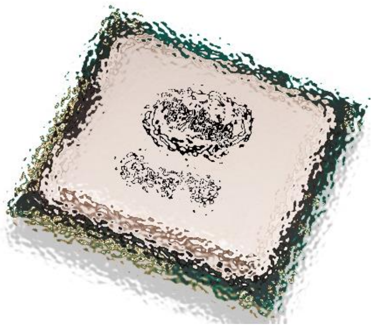


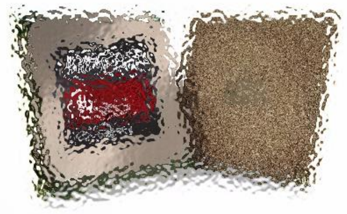
Active argument register
Global out-of-order tensor instruction queue:
Data prefetching/uploading, instruction dispatching, data reuse optimization
Domain-Specific Instructions
CPU-specific in-order queue
GPU-specific in-order queue
MIC-specific in-order queue
CPU
CPU
CPU
GPU
GPU
GPU
MIC
MIC
MIC
Remote data buffer
MAIN MEMORY
Data
Data

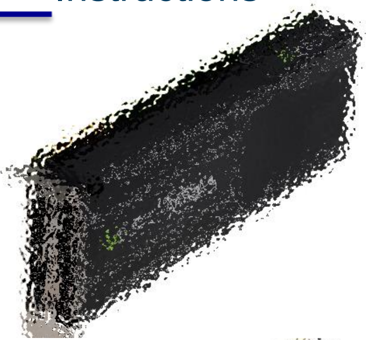






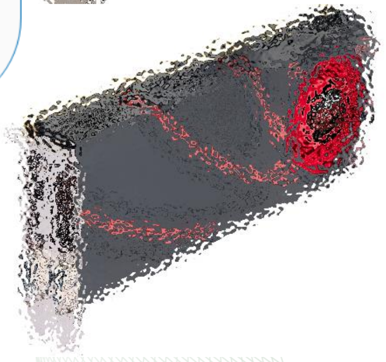
Node-Level Virtualization: Hiding Hardware

Domain-Specific Virtual Processor









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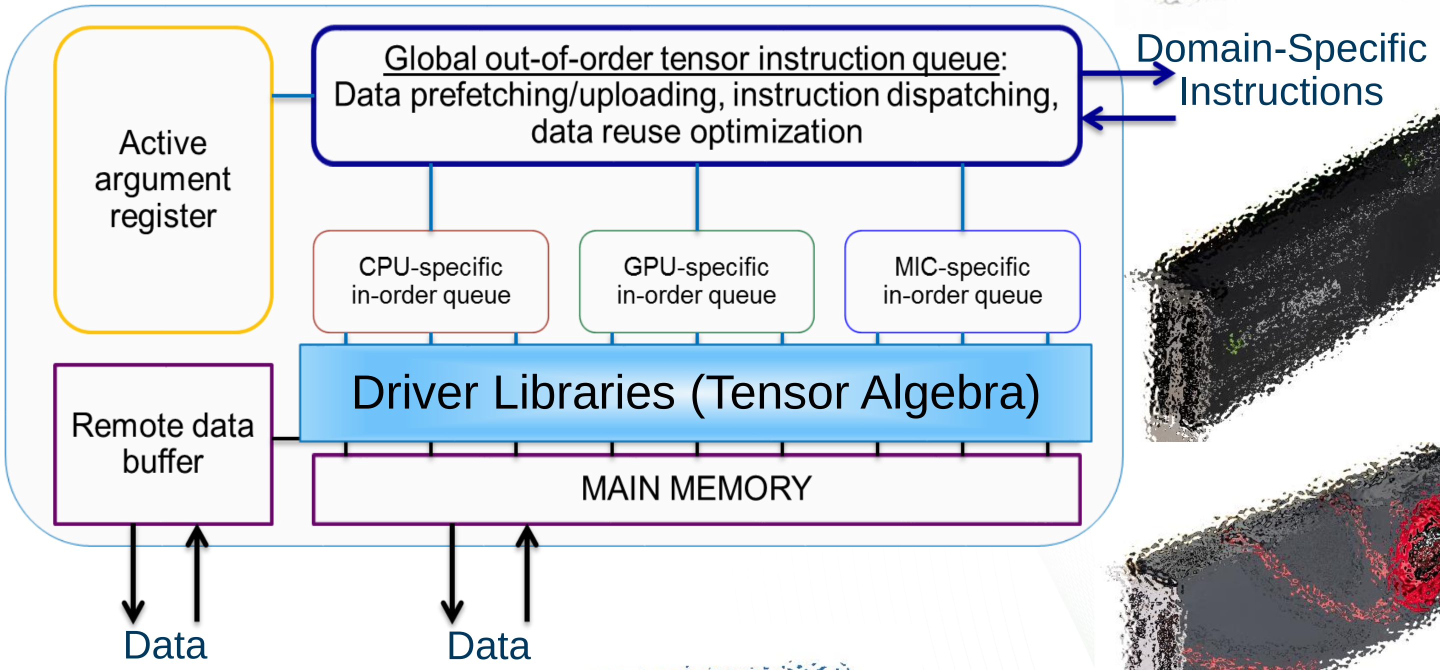
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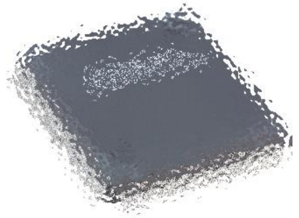
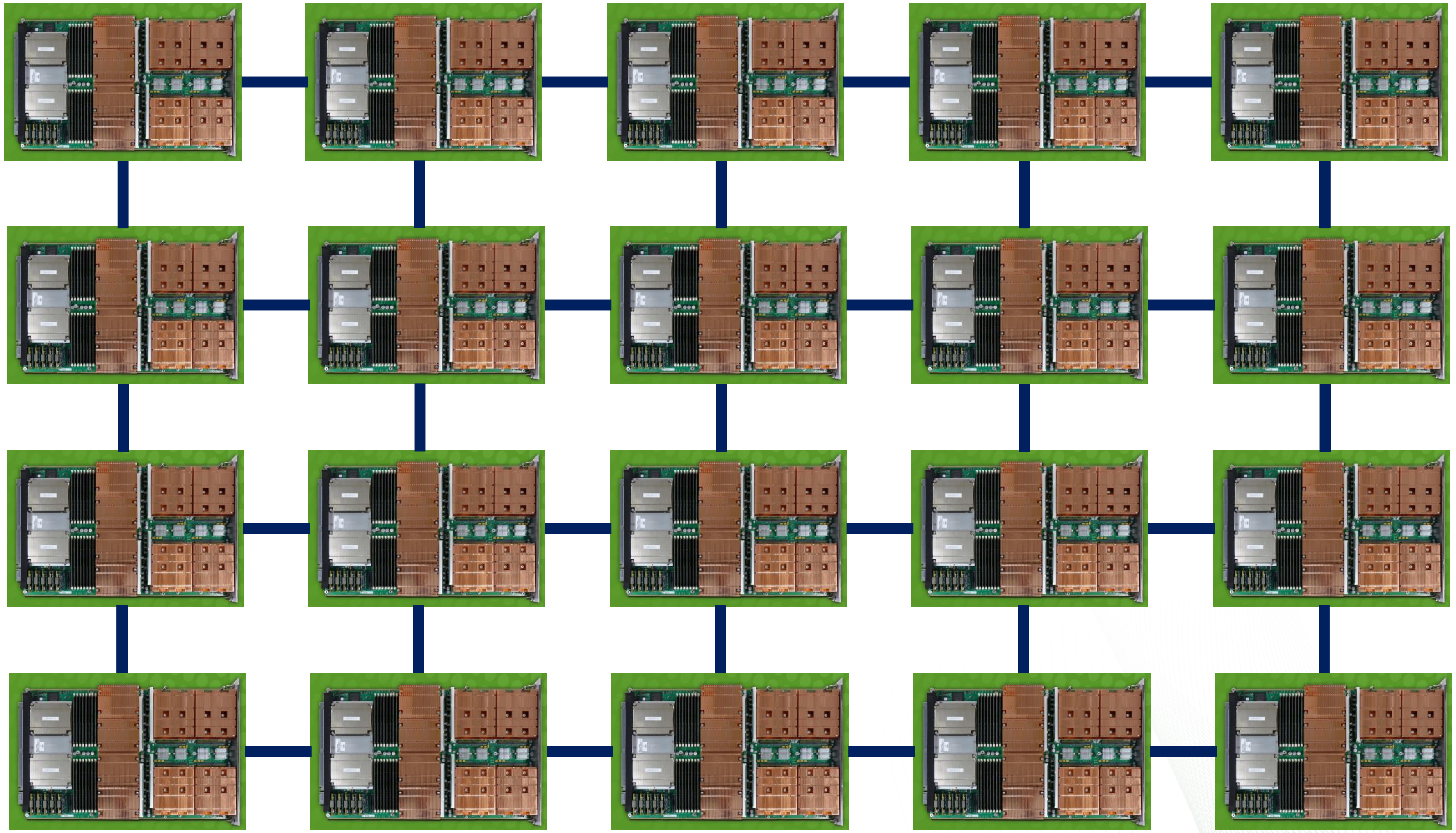
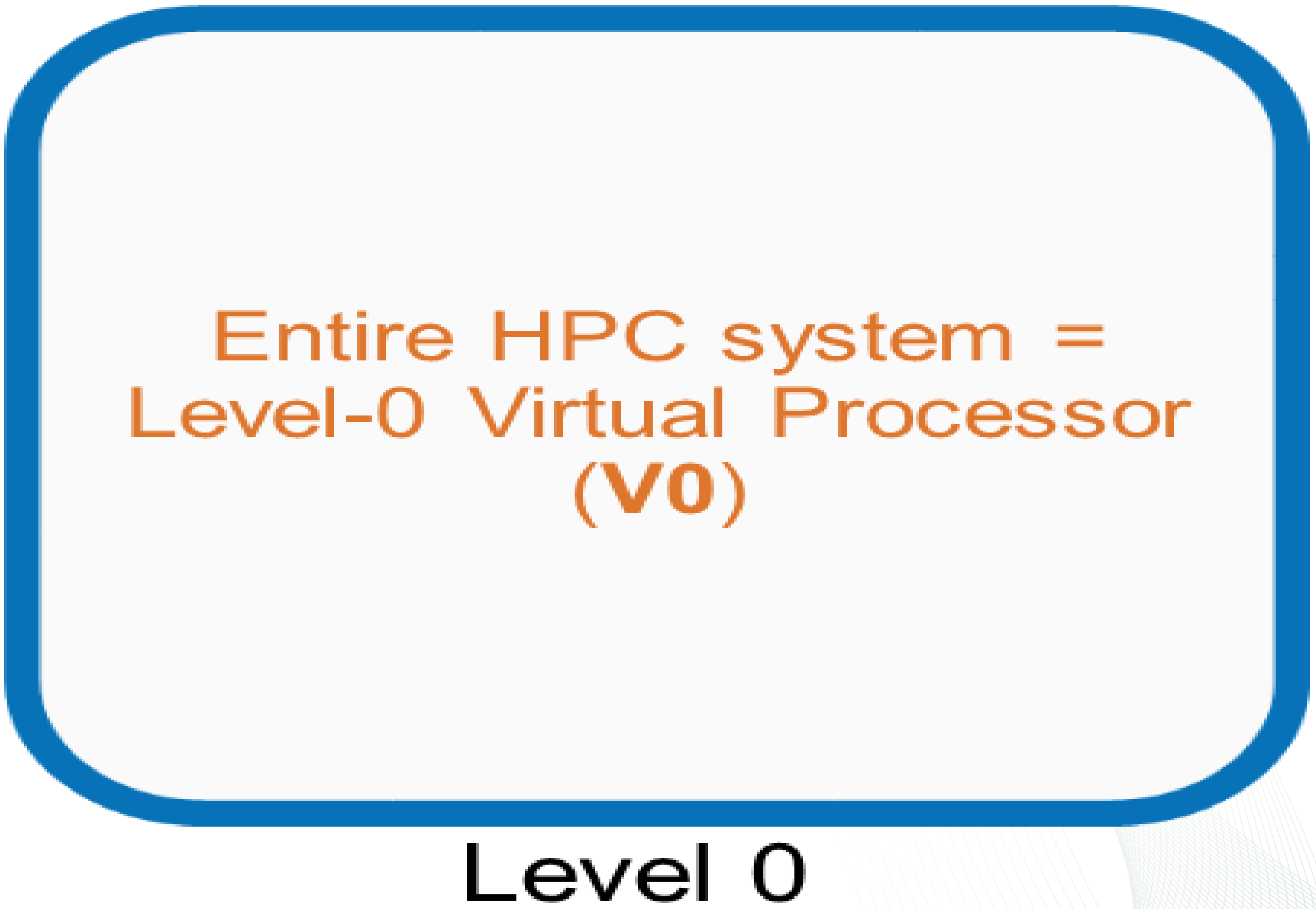


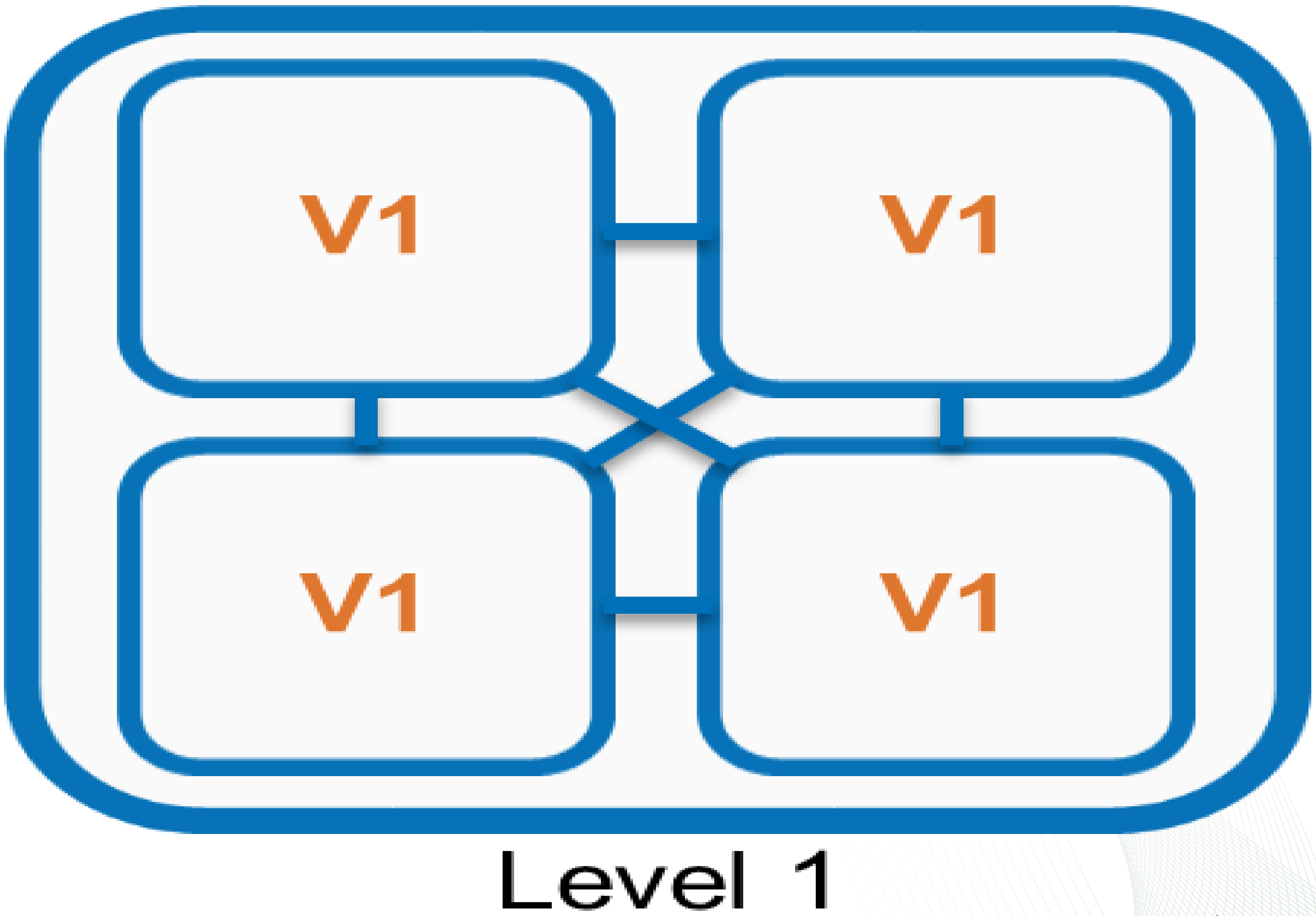
Global Virtualization: Hiding HPC Scale



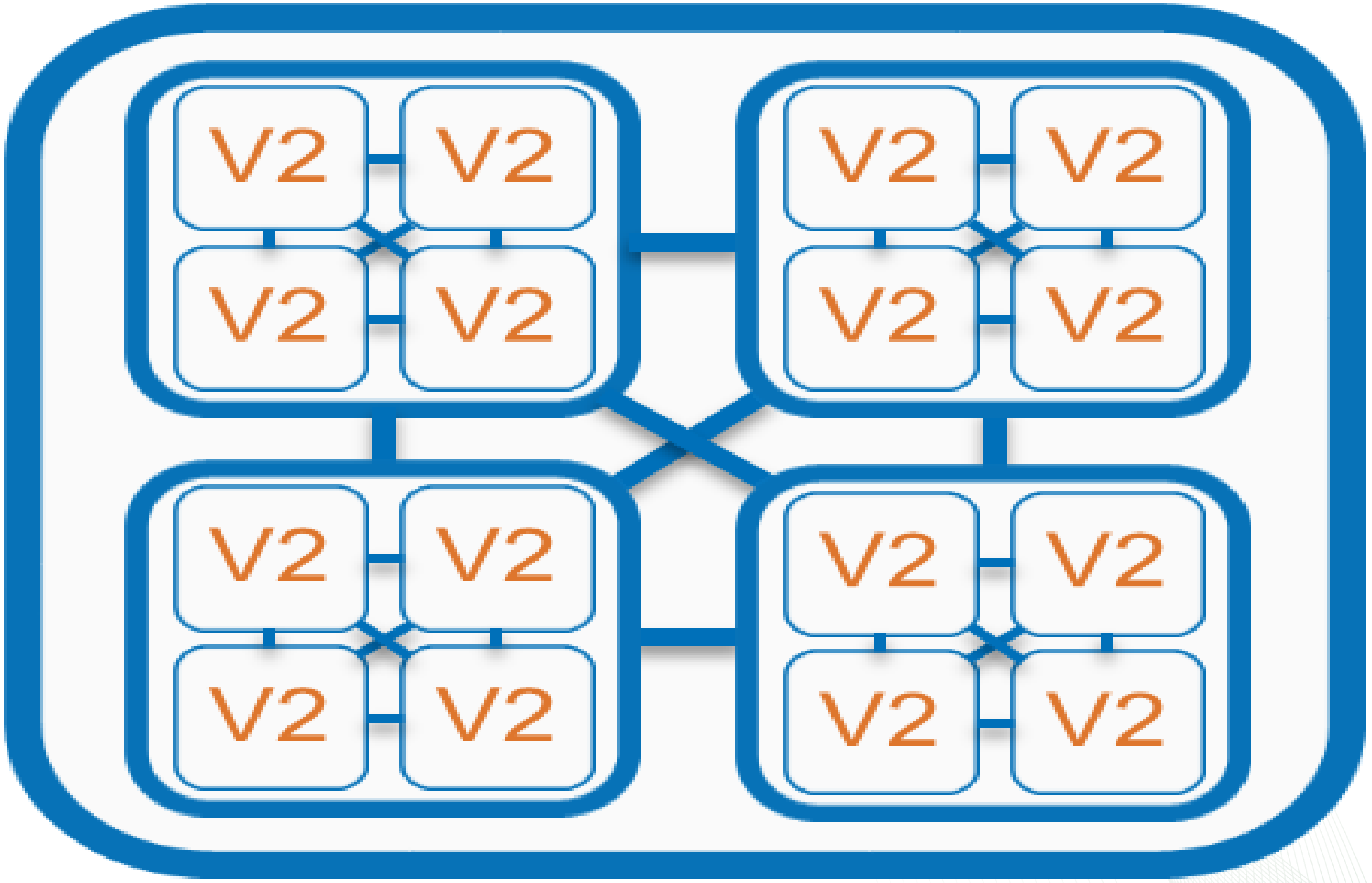
Global Virtualization: Hiding HPC Scale



Global Virtualization: Hiding HPC Scale

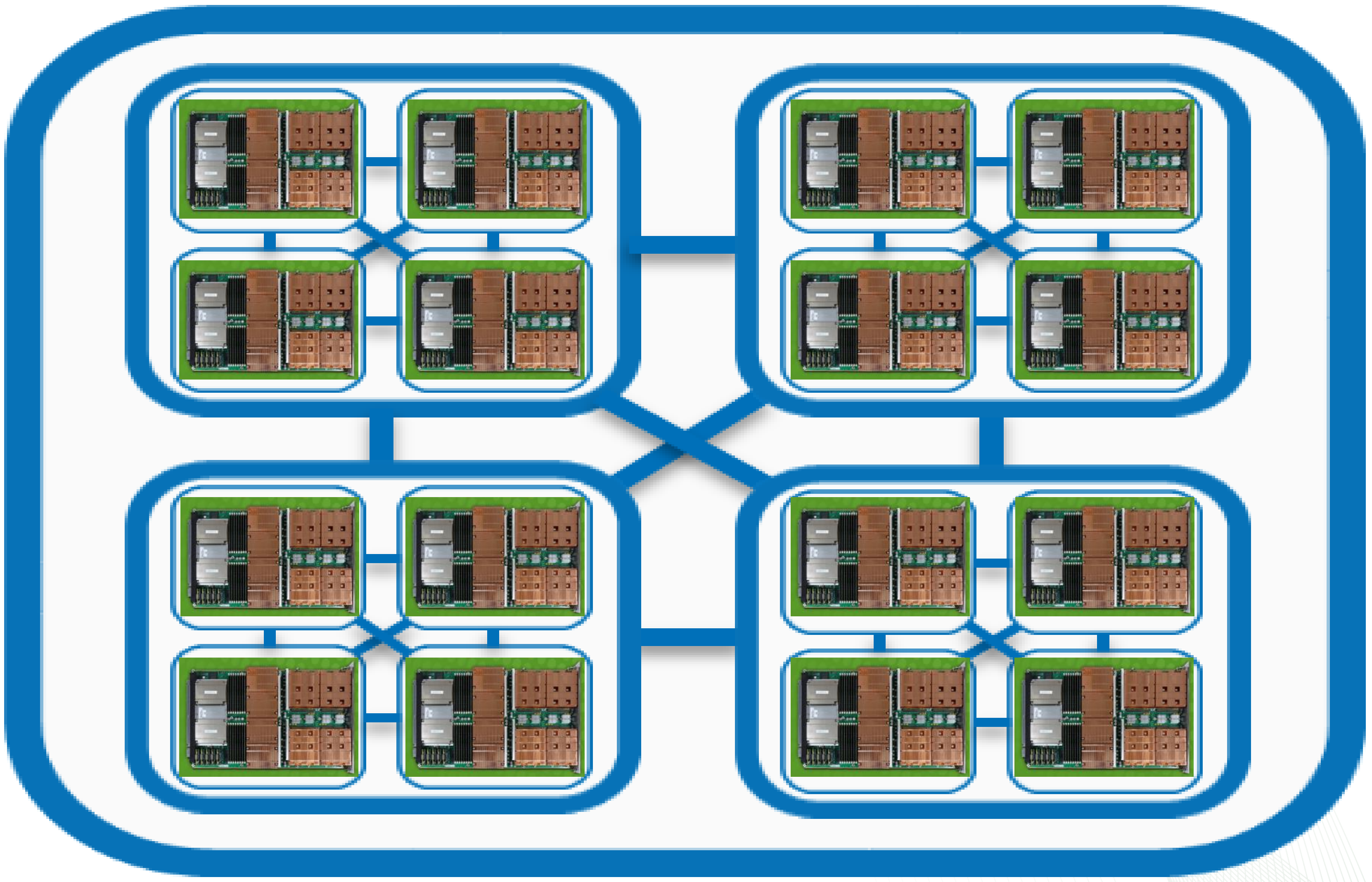


Global Virtualization: Hiding HPC Scale



Level 2

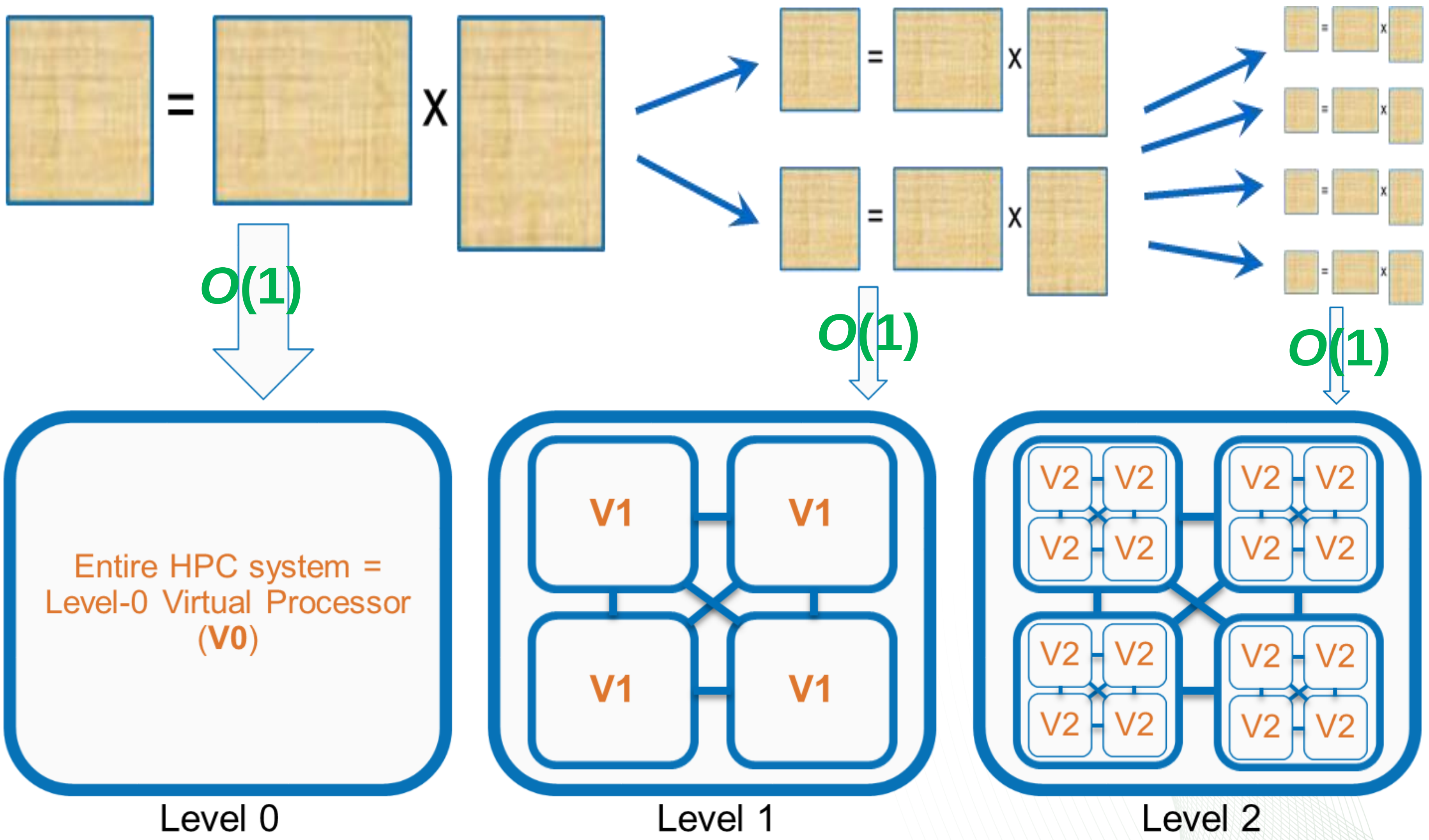
Global Virtualization: Hiding HPC Scale



Level 2

Recursive Dynamic Task Scheduling

Data storage granularity is decoupled from the task granularity



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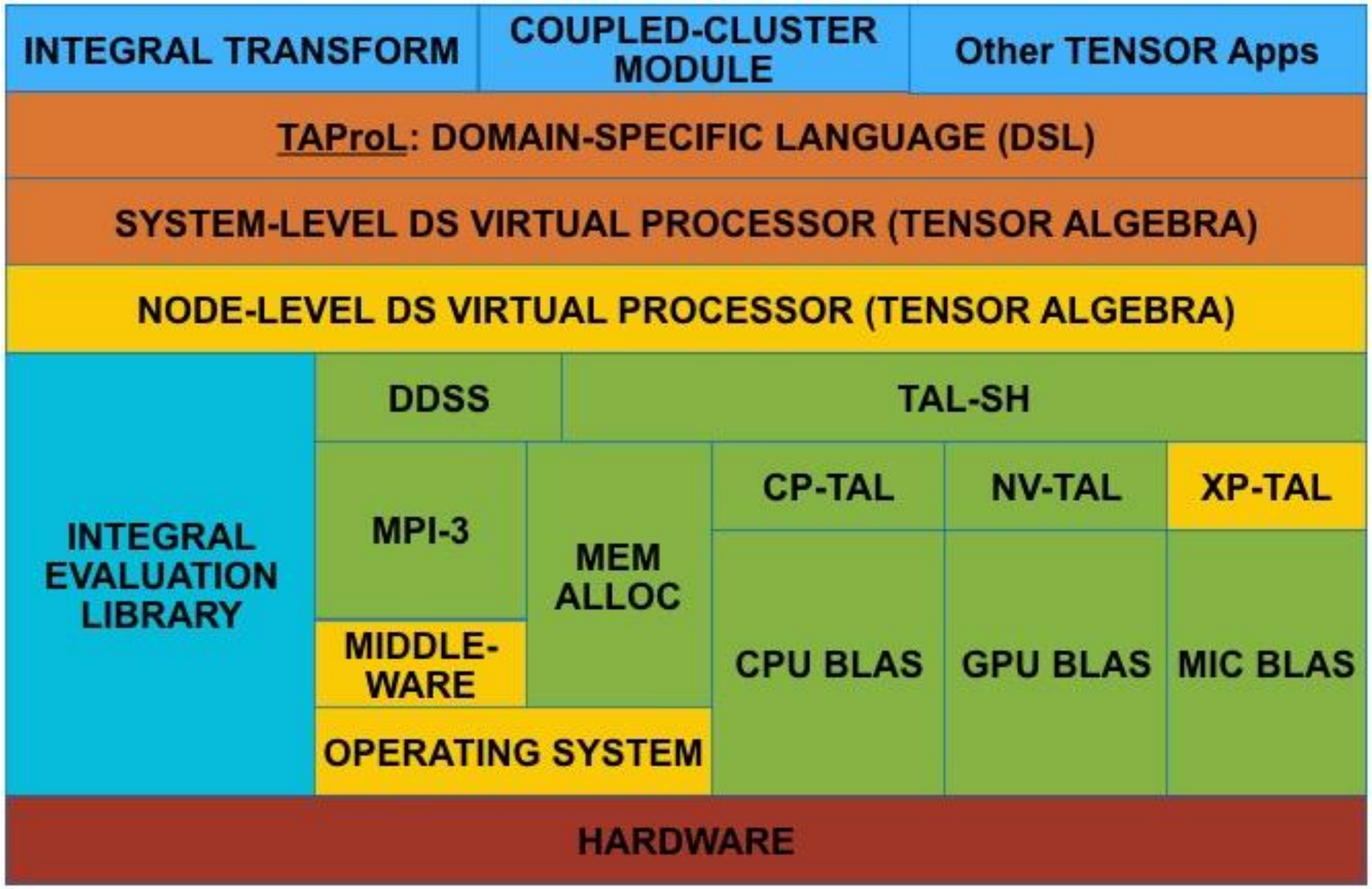
ExaTENSOR Software Layers

- Multi-component, library-based hierarchical framework for scalable tensor algebra, portable across different HPC platform: (CPU+ACC, Self-Hosted, …. Future?)


INTEGRAL TRANSFORM
COUPLED-CLUSTER MODULE
Other TENSOR Apps
TAProL: DOMAIN-SPECIFIC LANGUAGE (DSL)
SYSTEM-LEVEL DS VIRTUAL PROCESSOR (TENSOR ALGEBRA)
NODE-LEVEL DS VIRTUAL PROCESSOR (TENSOR ALGEBRA)
INTEGRAL EVALUATION LIBRARY
DDSS
TAL-SH
MPI-3
MEM ALLOC
CP-TAL
NV-TAL
XP-TAL
MIDDLE-WARE
CPU BLAS
GPU BLAS
MIC BLAS
OPERATING SYSTEM
HARDWARE

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TAL-SH: On-node Tensor Algebra Layer

- Basic tensor algebra operations: Tensor contraction, tensor product, tensor addition, tensor norm, etc.
- Supports multicore CPU and (multiple) NVIDA GPU
- Asynchronous execution on accelerators
- Automatic data transfer management and data transfer pipelining
- User-controlled data presence management
- Tensor contractions:
  - Up to 1.1 TFlop/s double precision on NVIDIA Kepler K20x for arithmetic intensities > 1000
  - Up to 4.1 TFlop/s double precision on NVIDIA Pascal P100 for arithmetic intensities > 1000

(Virtual) Conclusions

- Scalable, performance-portable tensor algebra via hardware and HPC scale abstraction:
  - Hardware agnostic by design;
  - HPC scale "agnostic" by design (still may require communication optimization);
  - Better fault-tolerance (virtual nodes can be turned on/off);
  - A good model for hardware/software co-design;
  - Easy to program, based on a domain-specific higher-level algorithm specification;
  - Better debugging (in terms of higher-level operations);
  - Better profiling (in terms of higher-level operations).
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