November 5, 2010

MPI at MPI

Jens Saak

Max Planck Institute for Dynamics of Complex Technical Systems
Computational Methods in Systems and Control Theory

MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

Parallel Computing Basics

Why Parallel Computing?

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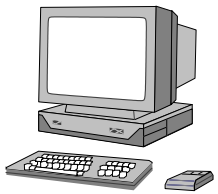
...all computations could be carried out on a single computer.

Parallel Computing Basics

Why Parallel Computing?

Then the world grew complicated and problems became large and difficult.



Parallel Computing Basics

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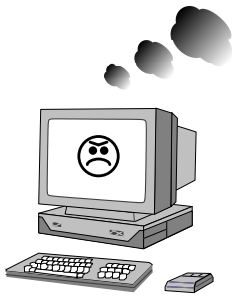

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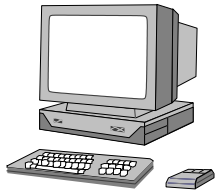

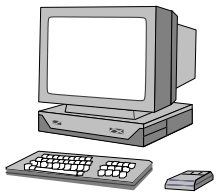

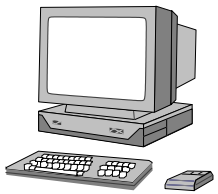

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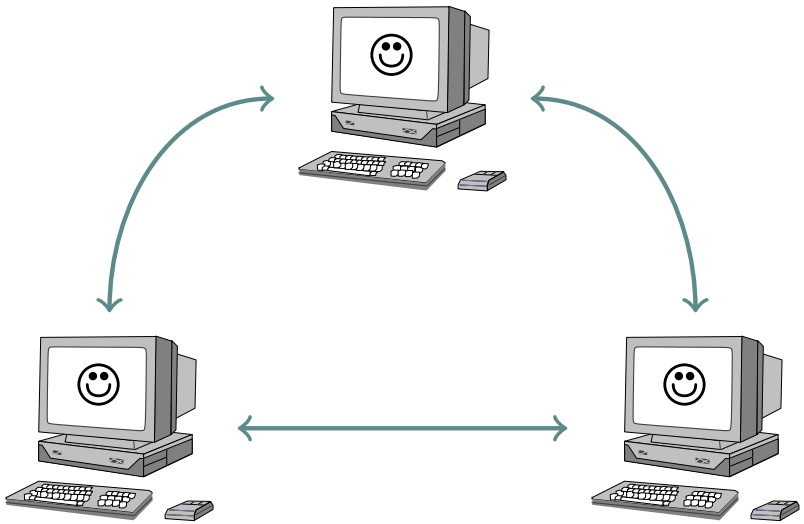

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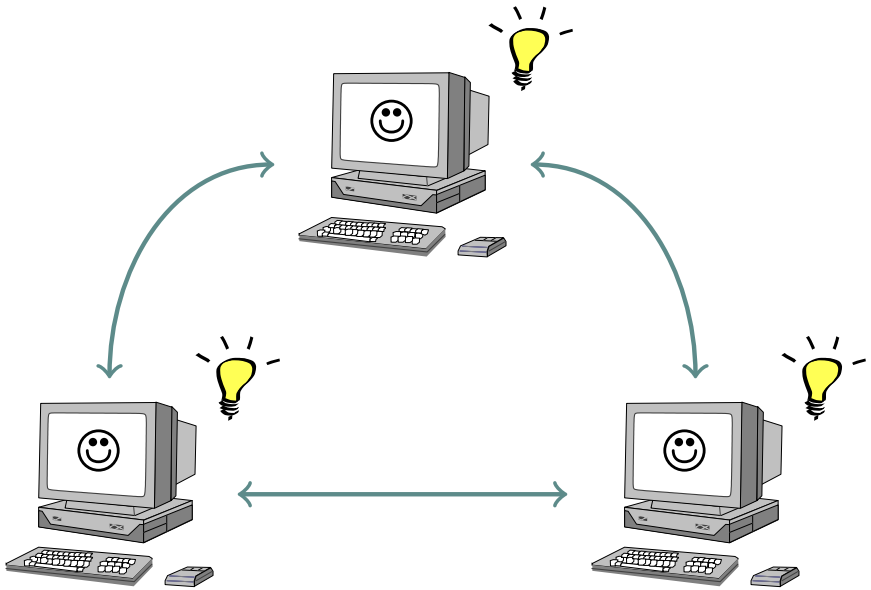

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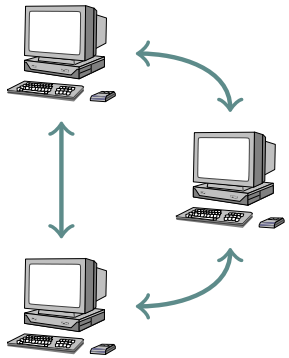
  computation on separate units with own memory on each unit



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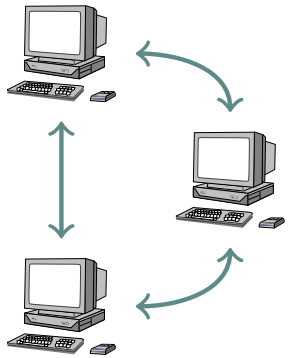
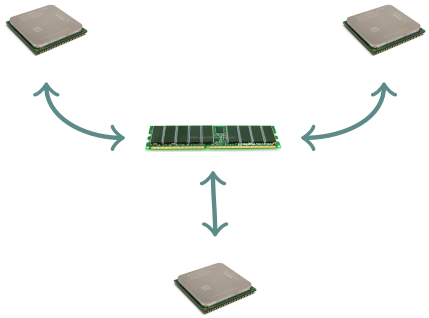


- Shared Memory Parallelism

  multiple computation units access a common memory



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  Data handling via the Message Passing Interface (MPI)

  (standard for a collection of operations and their semantics, NOT prescribing the actual protocol or implementation.)
  - MVAPICH/MVAPICH2 (implements MPI-1/MPI-2, BSD-License)
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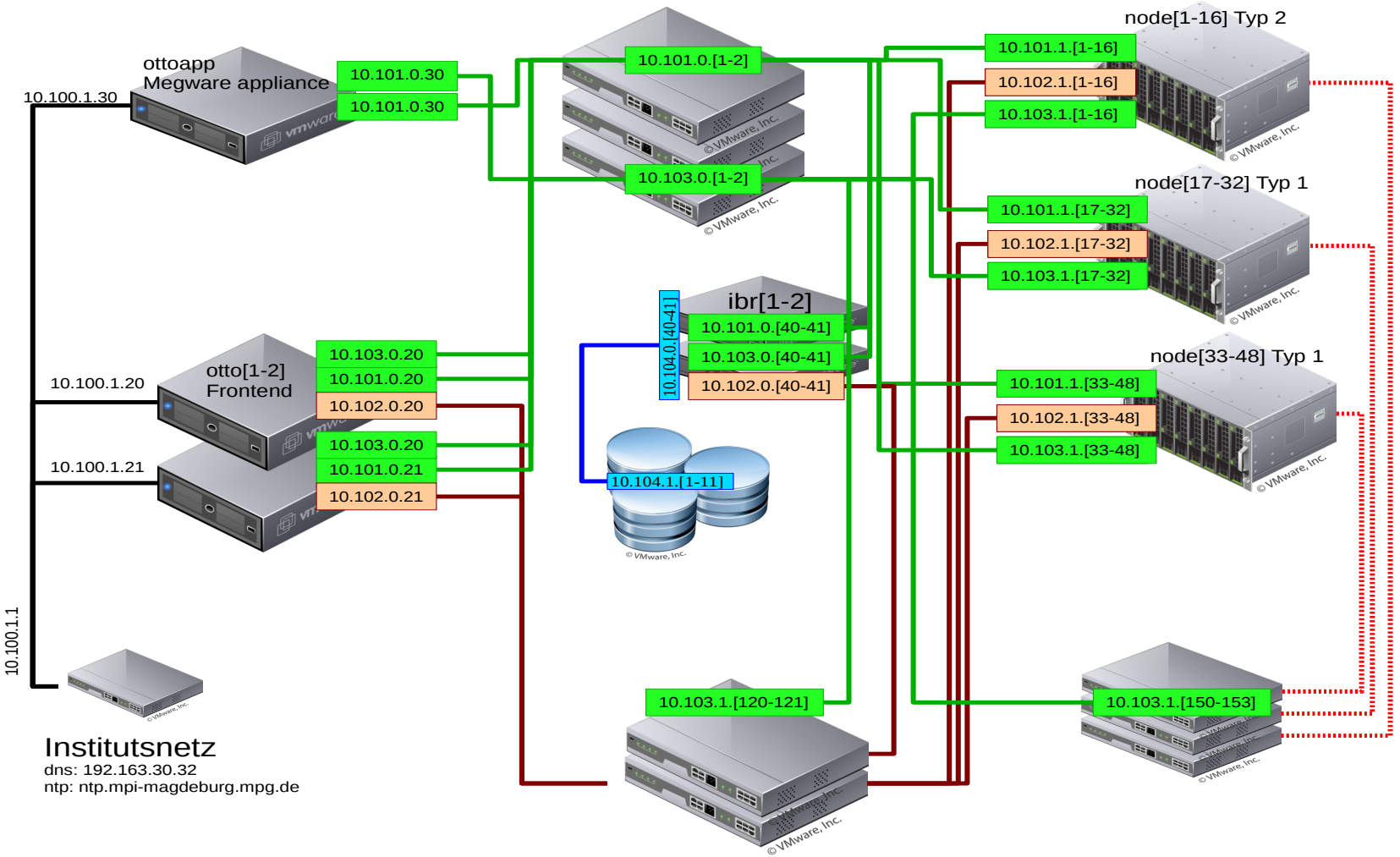
  OpenMP API: compiler and preprocessor directives. (latest version 3.0; May 2008)
  - GCC 4.3.2 and later
  - Intel Compilers 10.1 and later
  - Oracle, IBM, Cray, ...

Parallel Computing at MPI Magdeburg

otto



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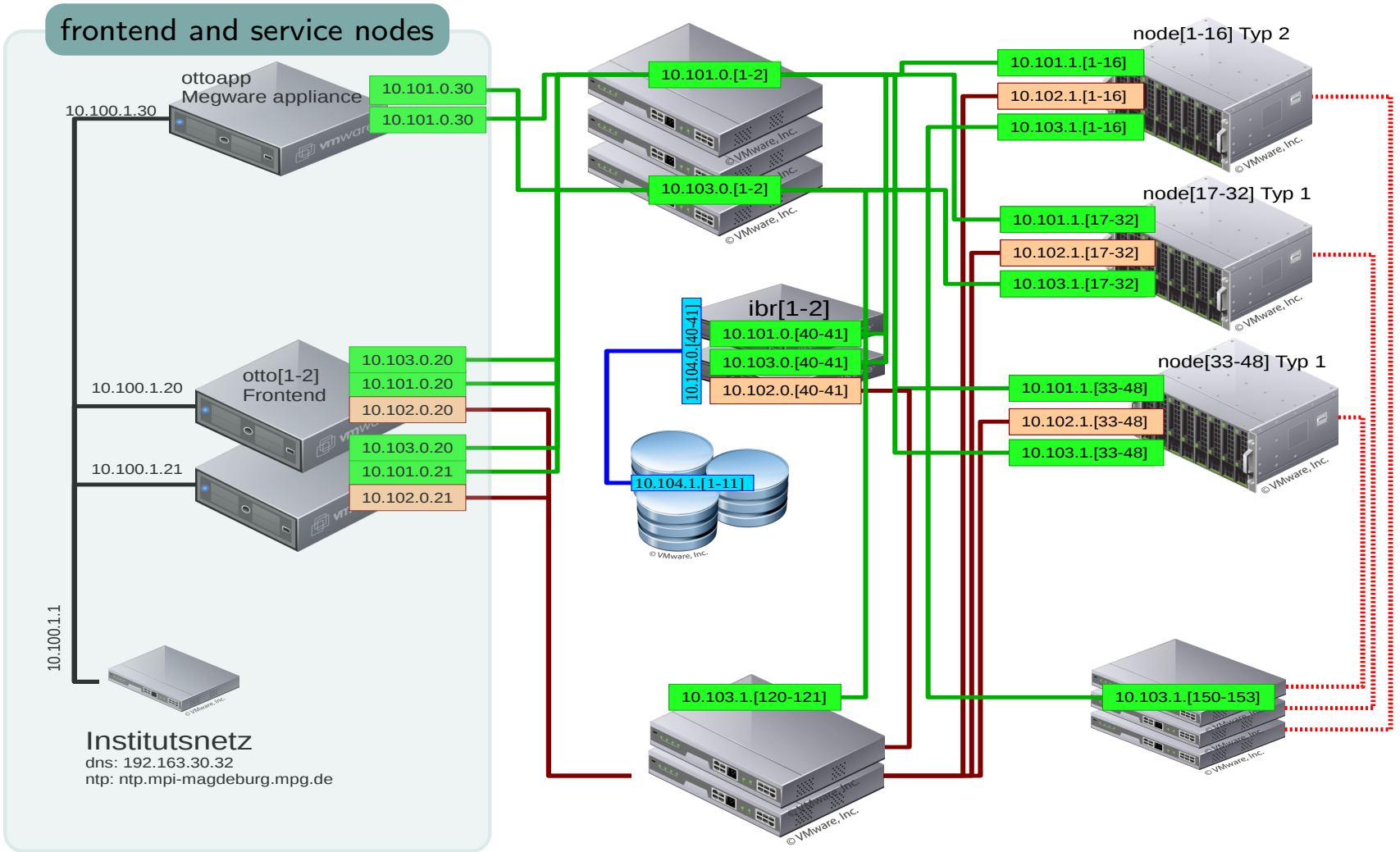

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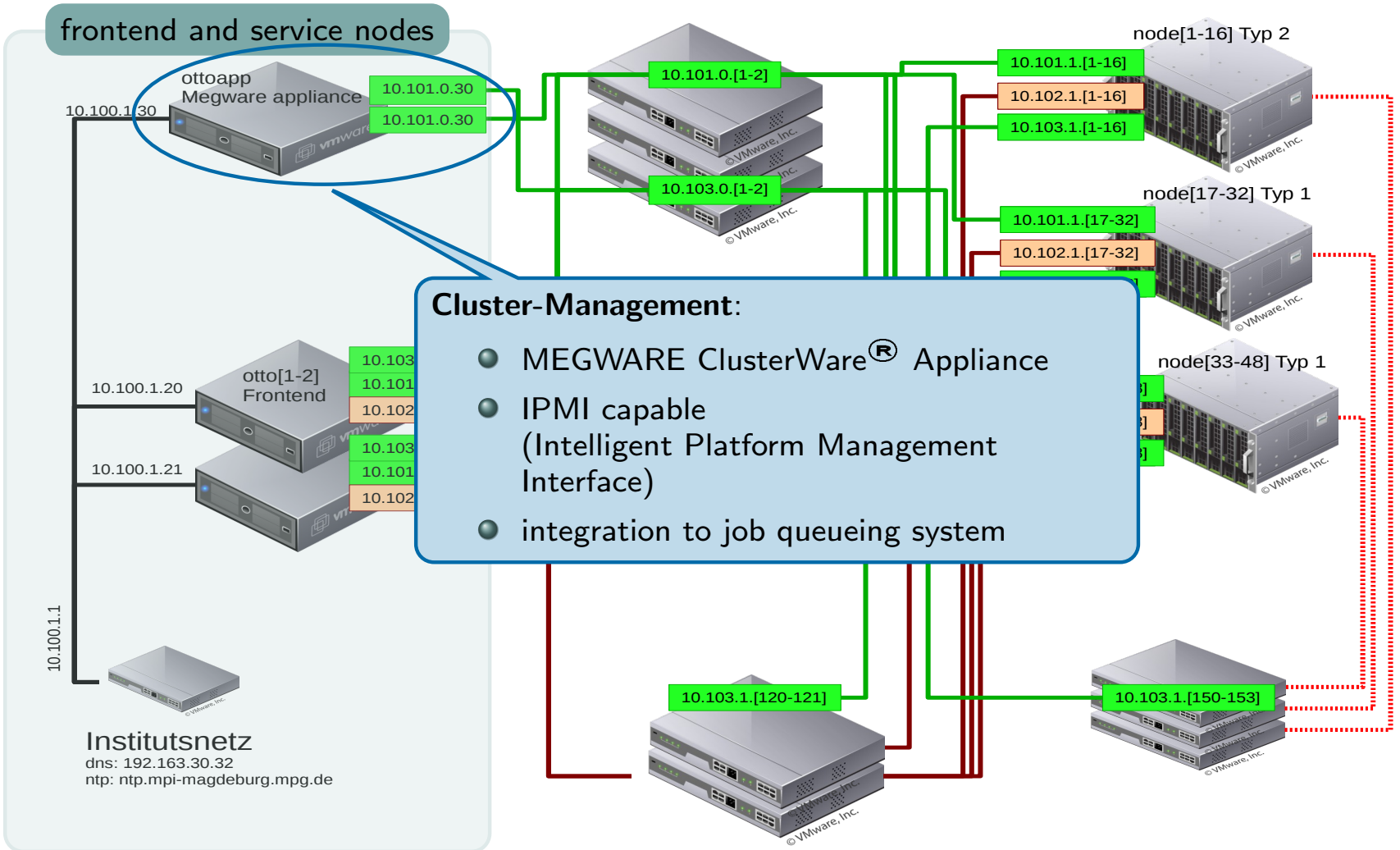

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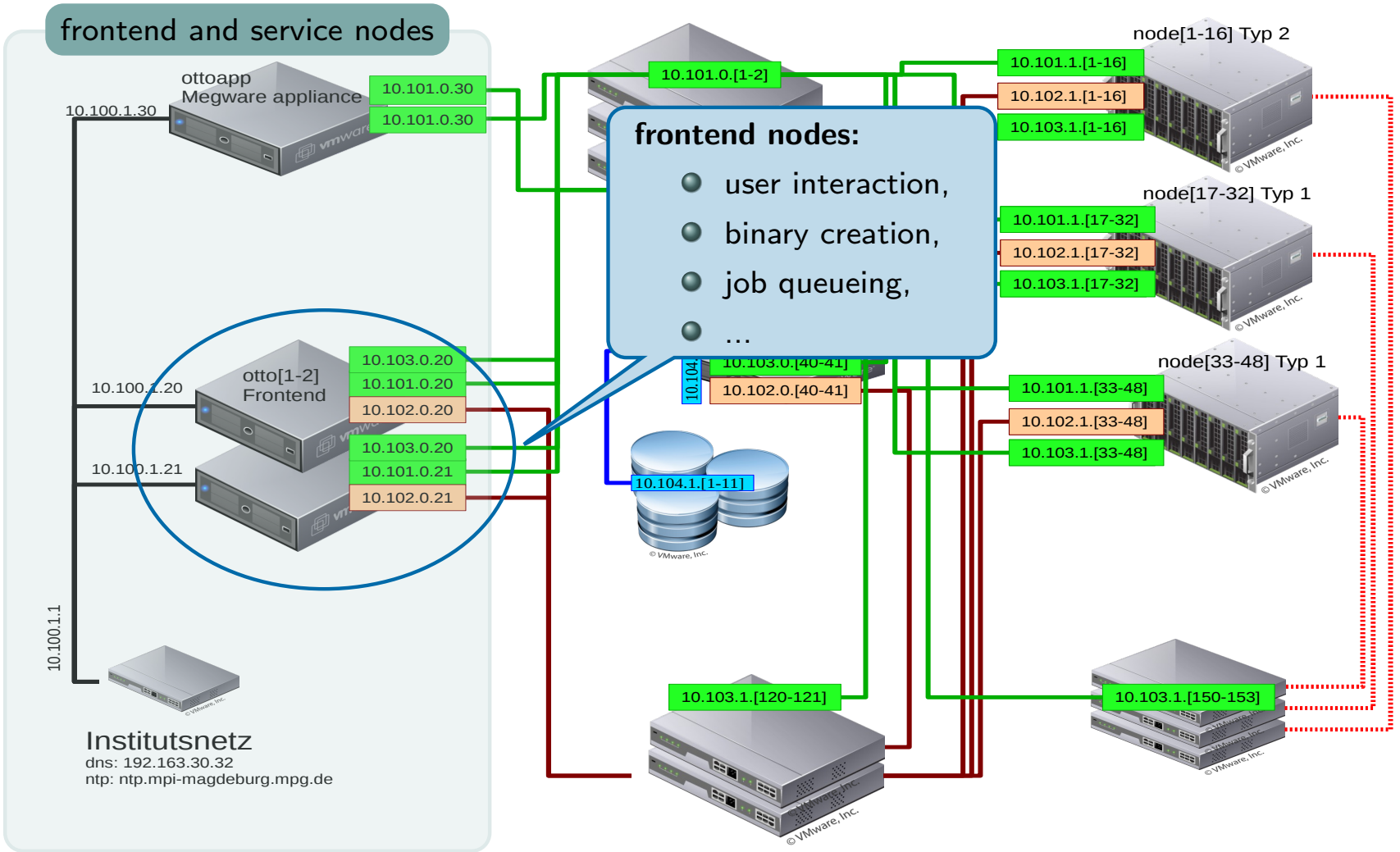

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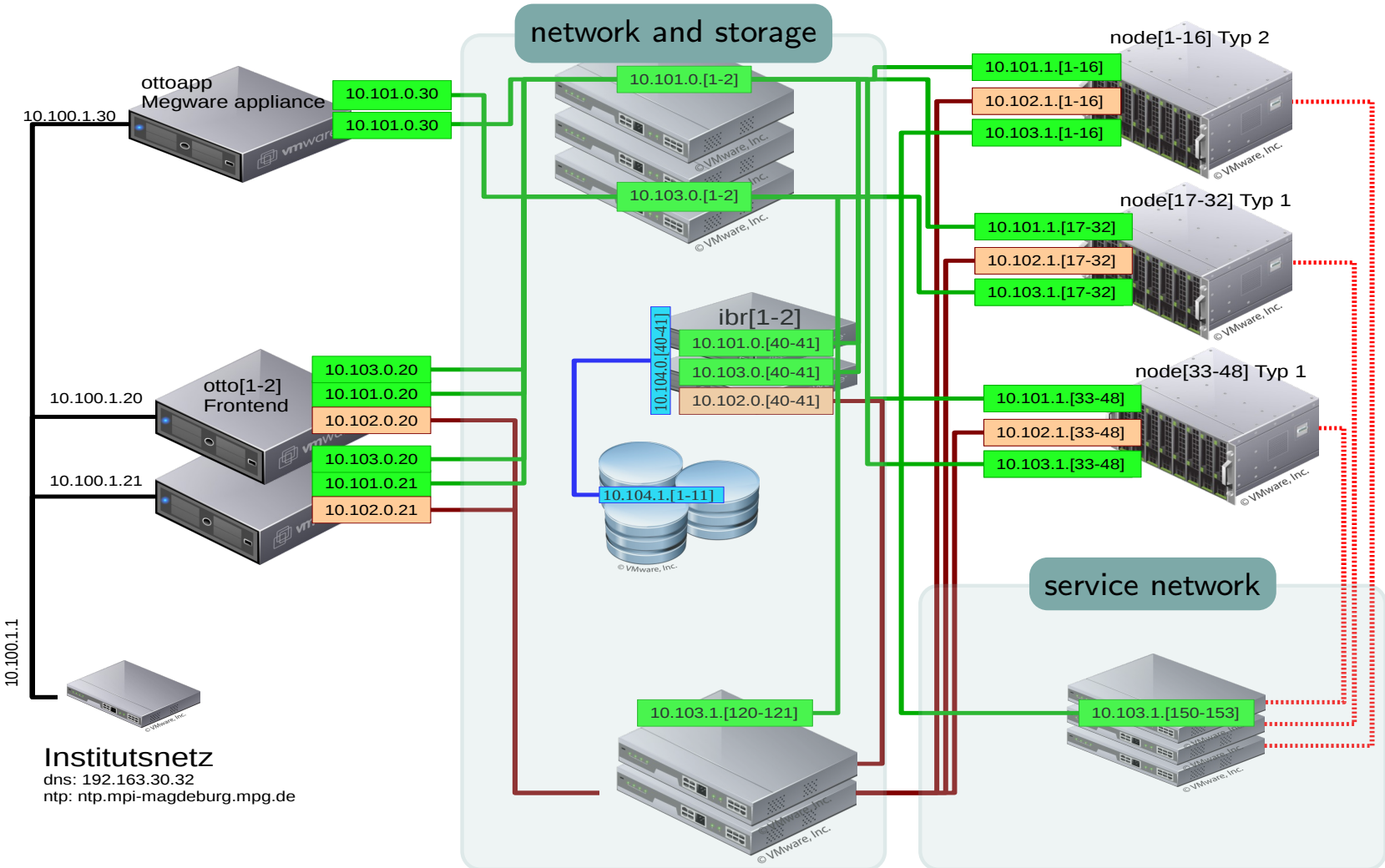

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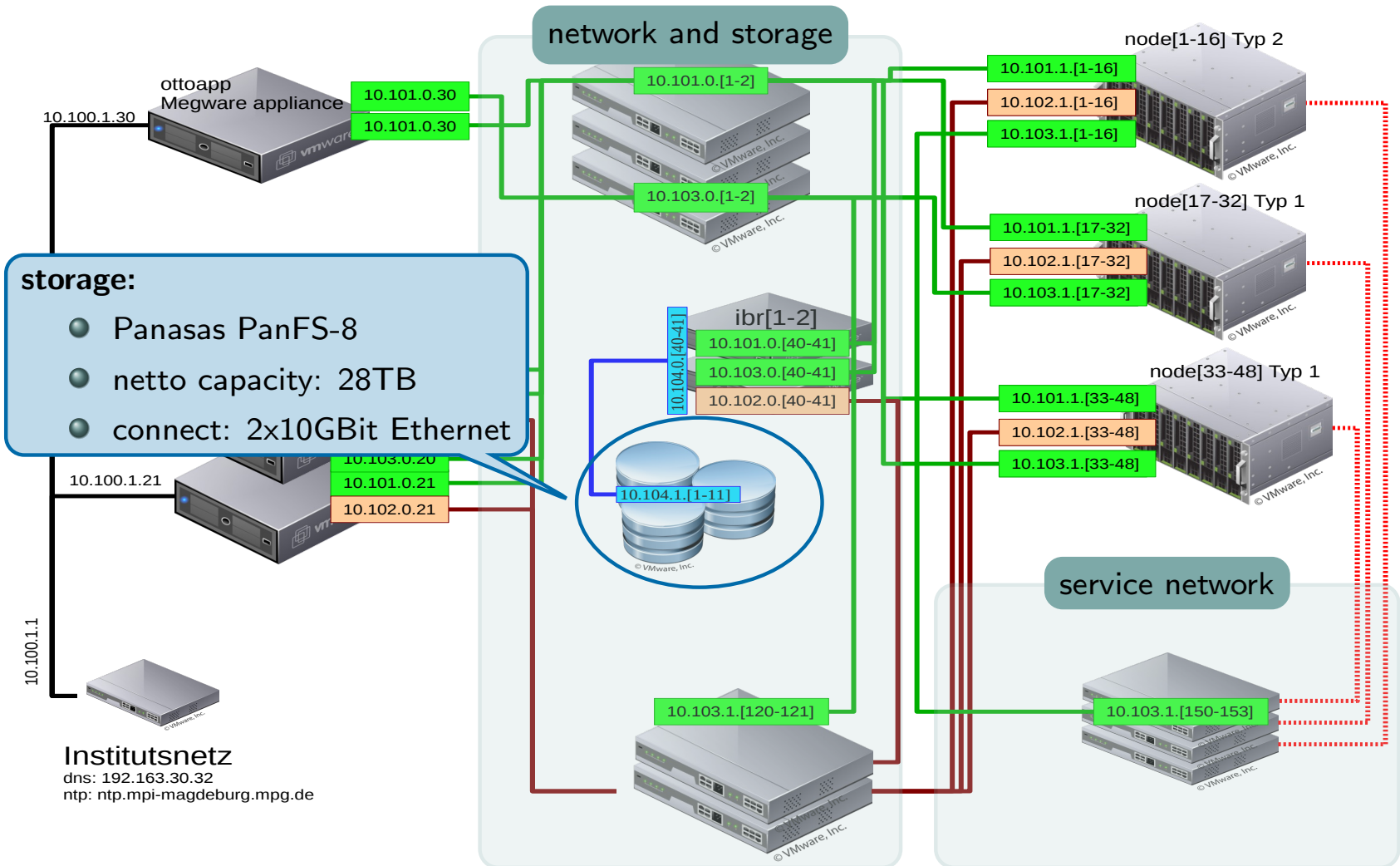

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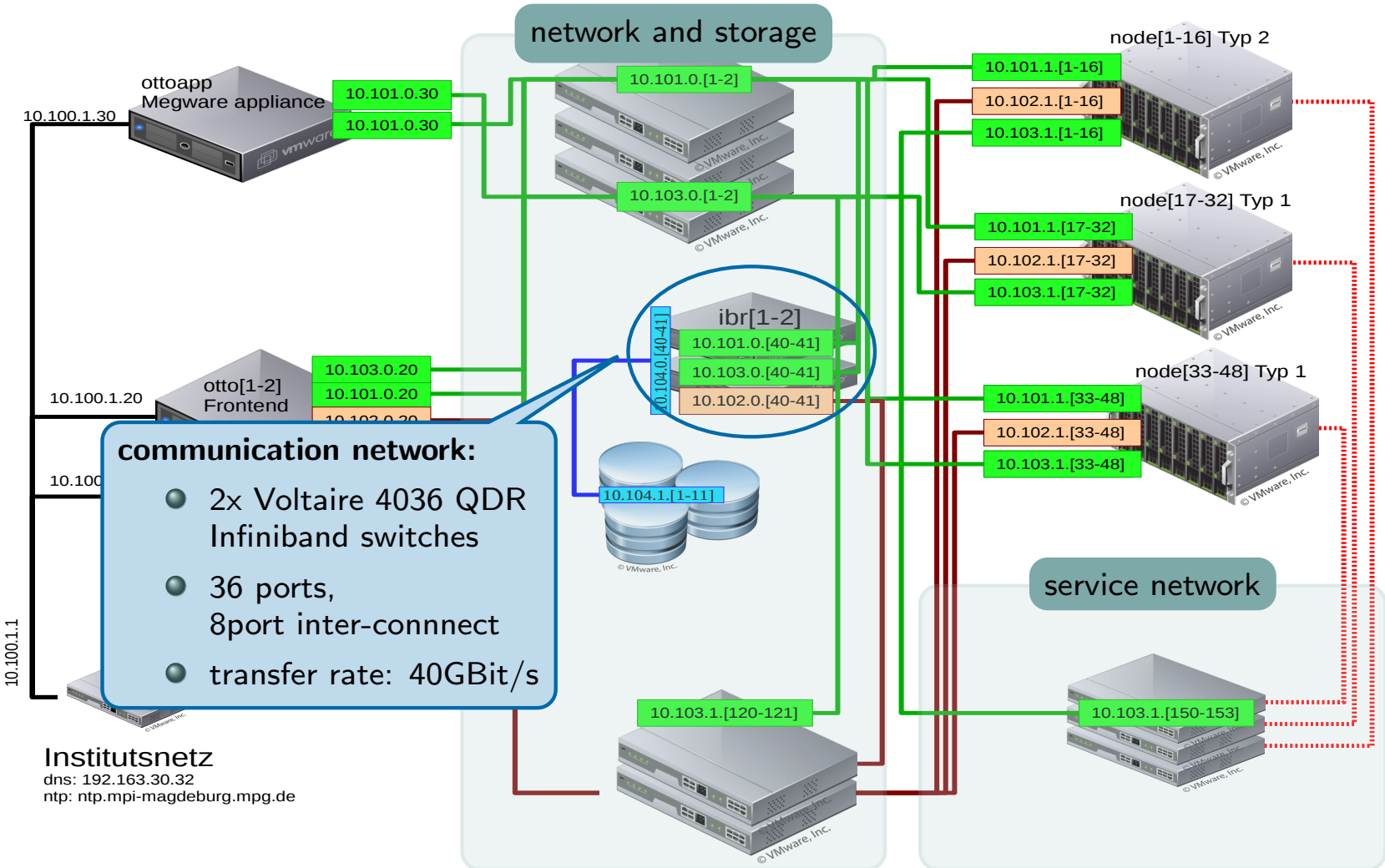

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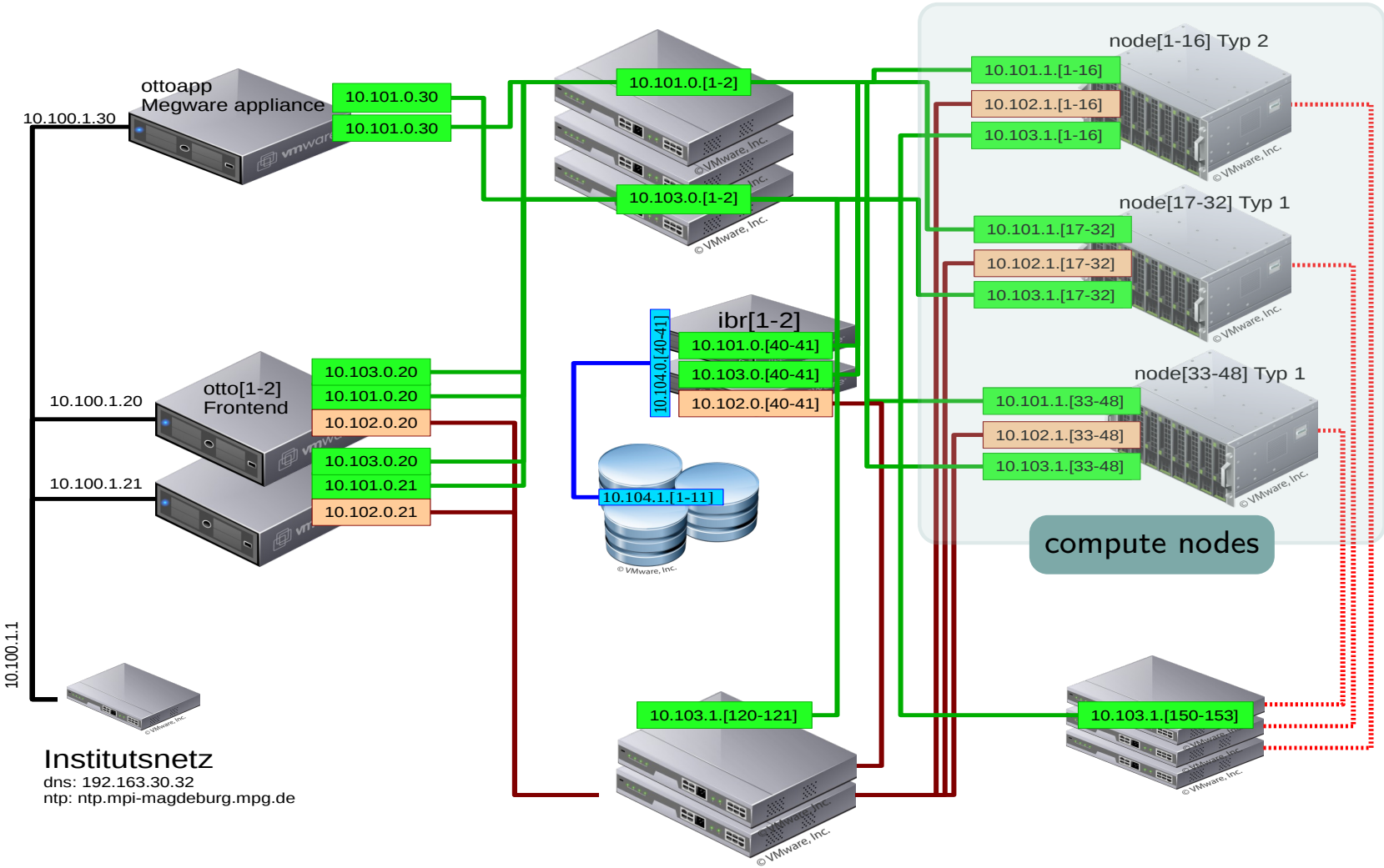

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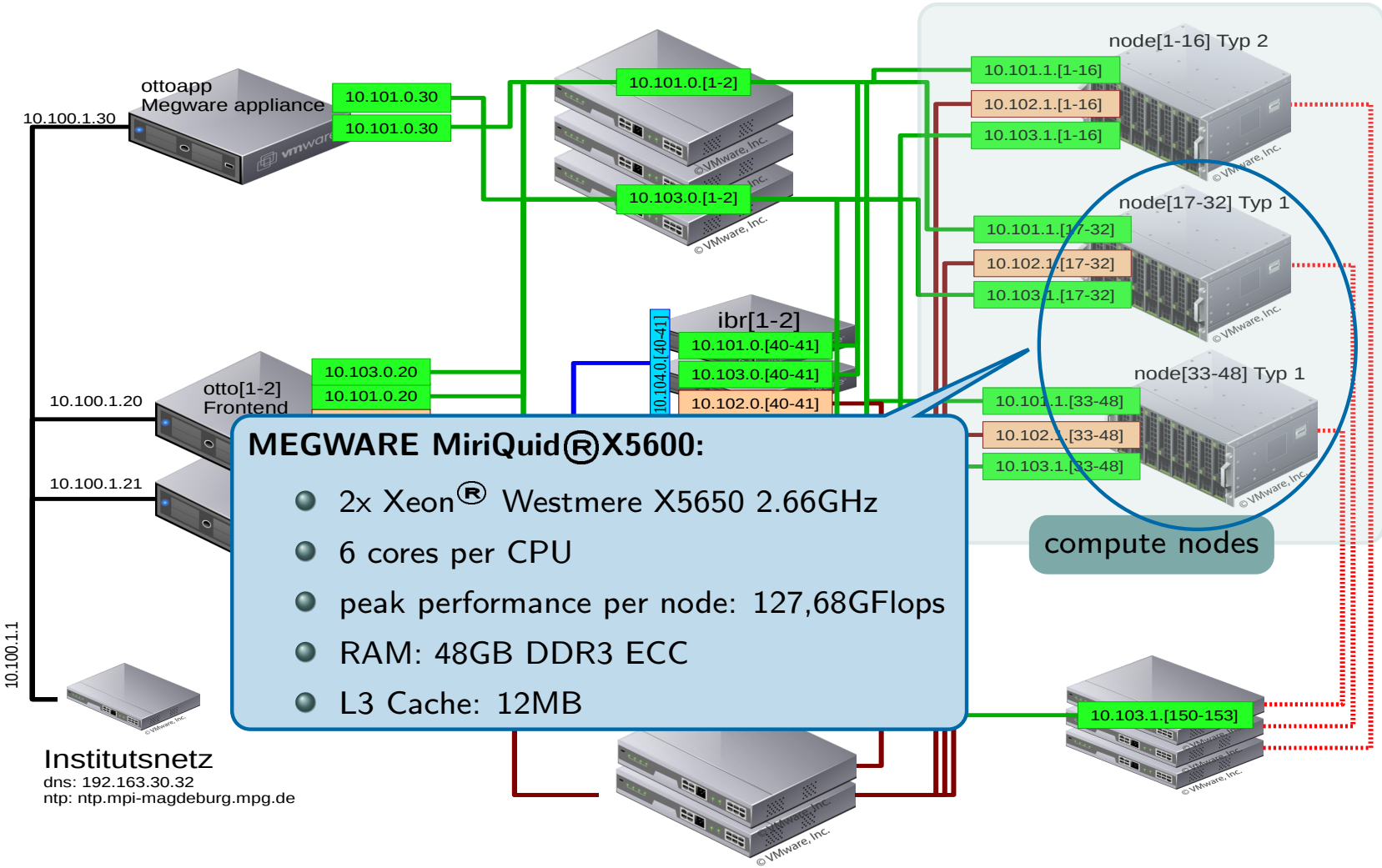

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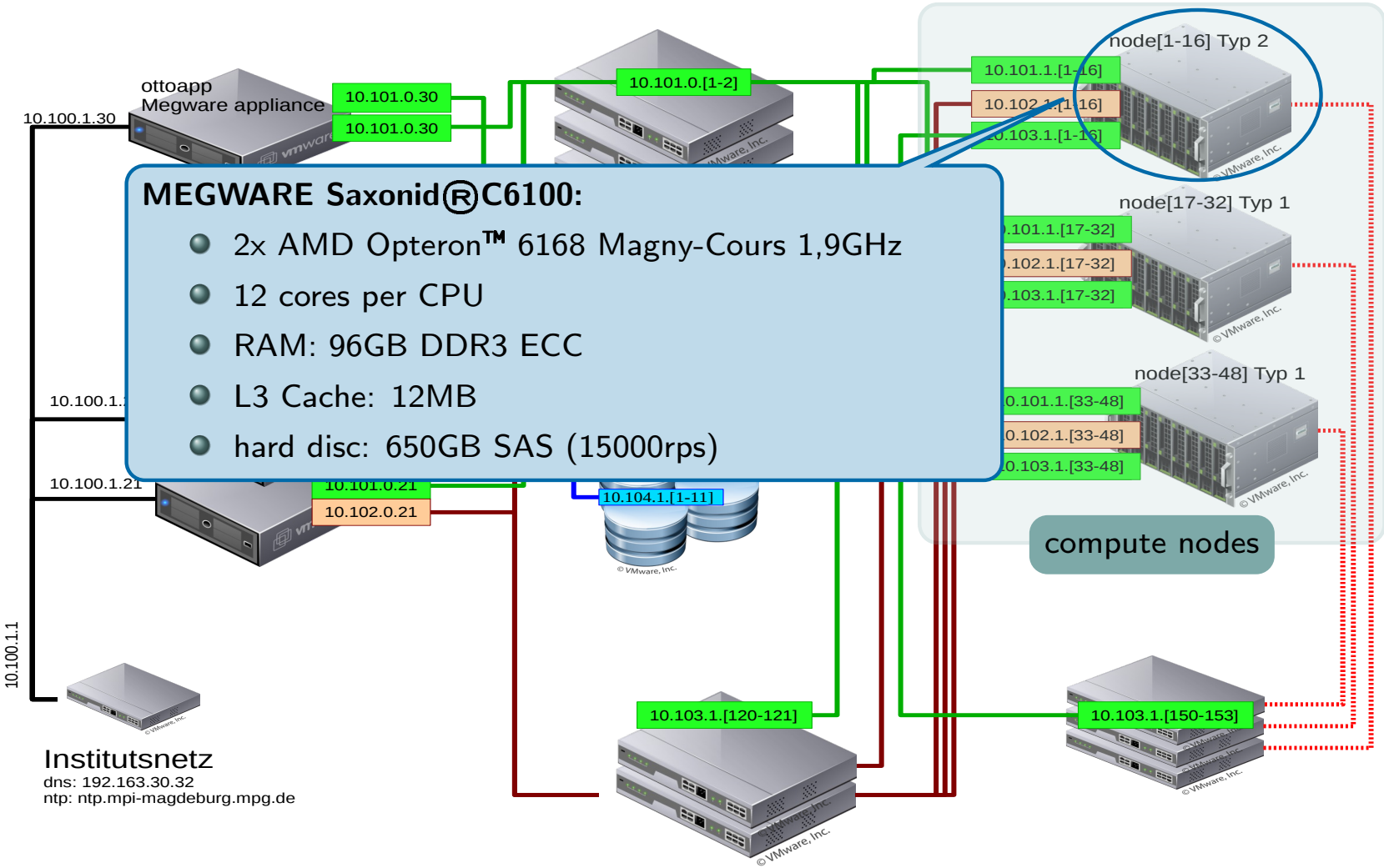

MEGWARE Saxonid®C6100:

- 2x AMD Opteron™ 6168 Magny-Cours 1,9GHz
- 12 cores per CPU
- RAM: 96GB DDR3 ECC
- L3 Cache: 12MB
- hard disc: 650GB SAS (15000rps)

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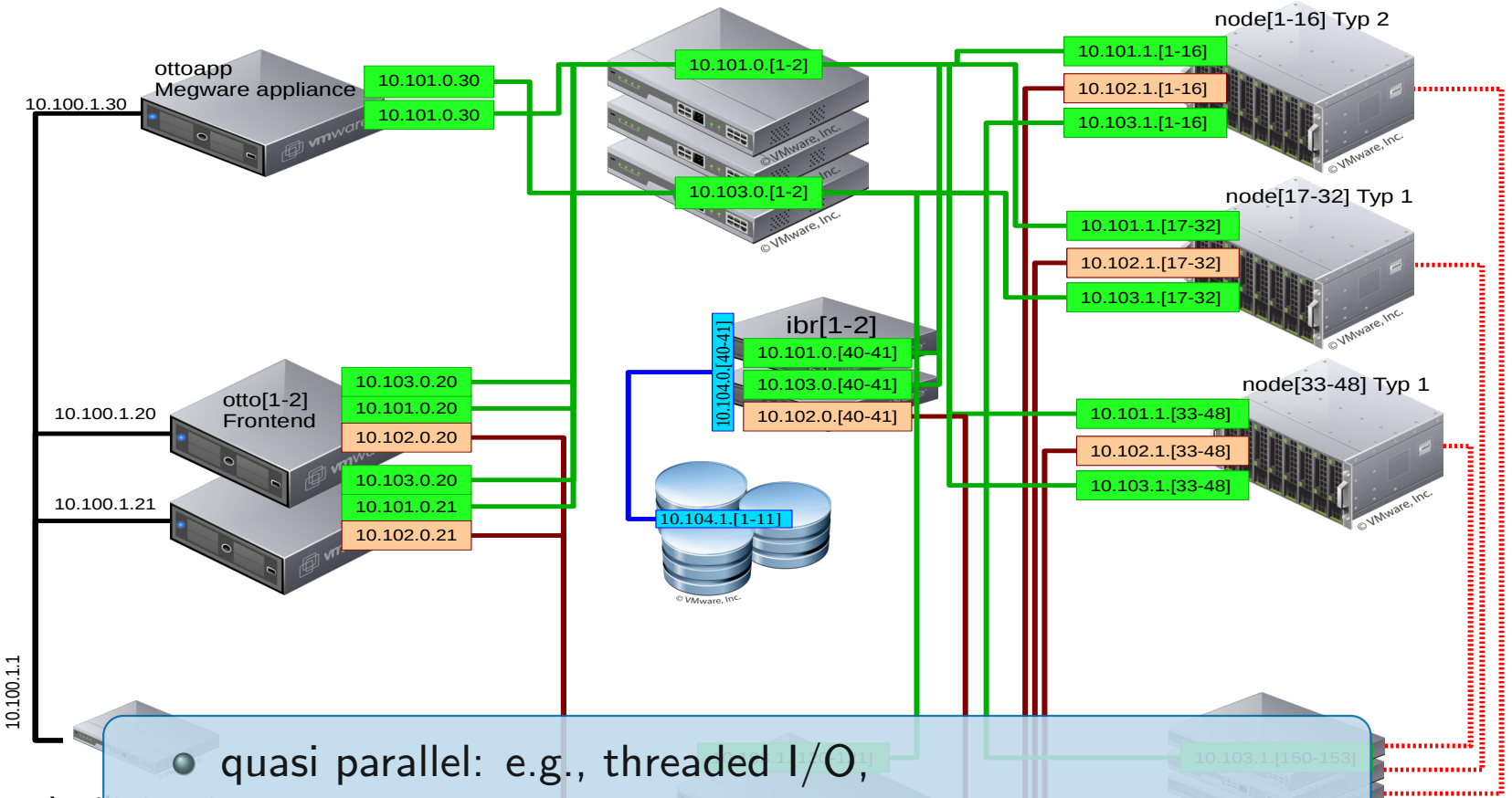

- quasi parallel: e.g., threaded I/O,
- distributed: every node has its own RAM,
- shared: 12/24 cores per node access the common RAM.

Parallel Computing at MPI Magdeburg

Molecular Simulations and Design

From wavefunctions to proteins in networks

The Molecular Simulations and Design (MSD) group aims at an explanation of chemical and biological phenomena at molecular level.

Complex phenomena in chemistry and biology

MSD group develops and applies tools from

- Quantum mechanics
- QM/MM hybrid simulations
- Molecular dynamics
- Brownian dynamics
- Bioinformatics
- Protein structural modeling

Contact: Dr. Matthias Stein

Parallel Computing at MPI Magdeburg

Computational Methods in Systems and Control Theory (CSC)

Interests:

Mathematical methods for application in systems and control theory and their numerical realization, with focus on Numerical Linear Algebra.

Parallel Computing:

- accelerate solvers on modern multi-core processors
- solve very large
  - matrix equations,
  - model order reduction problems,
  - or optimal control problems

  on high performance parallel machines.

Parallel Computing aware Software developed in CSC:

- PLiCMR
- C.M.E.S.S.

Parallel Computing in CSC

PLiCMR

Parallel Library in Control and Model Reduction.

http://www.pscom.uji.es/modred/index.html

Distributed memory parallel model order reduction via

- Balanced Truncation
- Singular Perturbation Approximation
- Hankel-Norm Approximation

Partners: High Performance Computing and Architectures Group
(University Jaume I; Castellón; Spain)
http://www.hpca.uji.es/

Parallel Computing in CSC

C.M.E.S.S.

C-language **M**atrix **E**quation **S**parse **S**olver

C-Library for solving large sparse:

- Lyapunov equations
  $\mathbf{FX} + \mathbf{XF}^T = -\mathbf{GG}^T, \qquad \mathbf{FXE}^T + \mathbf{EXF}^T = -\mathbf{GG}^T,$

See poster, as well.

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  - Balanced Truncation (first and second order systems)
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Currently focused on multi-core desktop computers, i.e., shared memory.

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> “...and they all computed happily ever after.”