ITEA 2

INFORMATION TECHNOLOGY FOR EUROPEAN ADVANCEMENT

How to Accelerate an Application: A Practical Case Study in Combustion Modelling

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Parallel Programming for Multi-core Architectures

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Combustion Modelling Software

- **The Combustion Modelling Software RECOM-AIOLOS is a tailored application for the mathematical modelling of industrial firing systems ranging from several hundred kW to more than 1000 MW.**

- **The Software solves approx. 100 conservation equations (mass, momentum, energy, species concentrations, radiation) on a 10-15 million cells finite volume grid, leading to high computational demands.**

- **The Software, originally designed for High-Performance Computing on Parallel Vector-Computers and Massively Parallel Systems, has been ported to low-cost Multi-Core systems to expand the hardware base.**

- **A Suite of Optimization Tools (MARMOT, VAMPIR, SCALASCA, MAQAO) was used for Performance Tuning to identify performance bottlenecks and potential improvements in a systematic way.**

Applied Workflow

- **High Level Performance Analysis of existing MPI-Parallelization**
  - Checking of MPI-Implementation with the Tool MARMOT
  - Analysing MPI-Parallel Execution with the Tools VAMPIR & SCALASCA

    ➡ Optimized massively parallel execution across nodes

- **Low Level Performance Analysis for single and multi core**
  - Checking single and multi core execution on subroutine level using performance counters (VAMPIR / MAQAO)
  - Checking performance bottlenecks on loop level within critical subroutines (MAQAO)

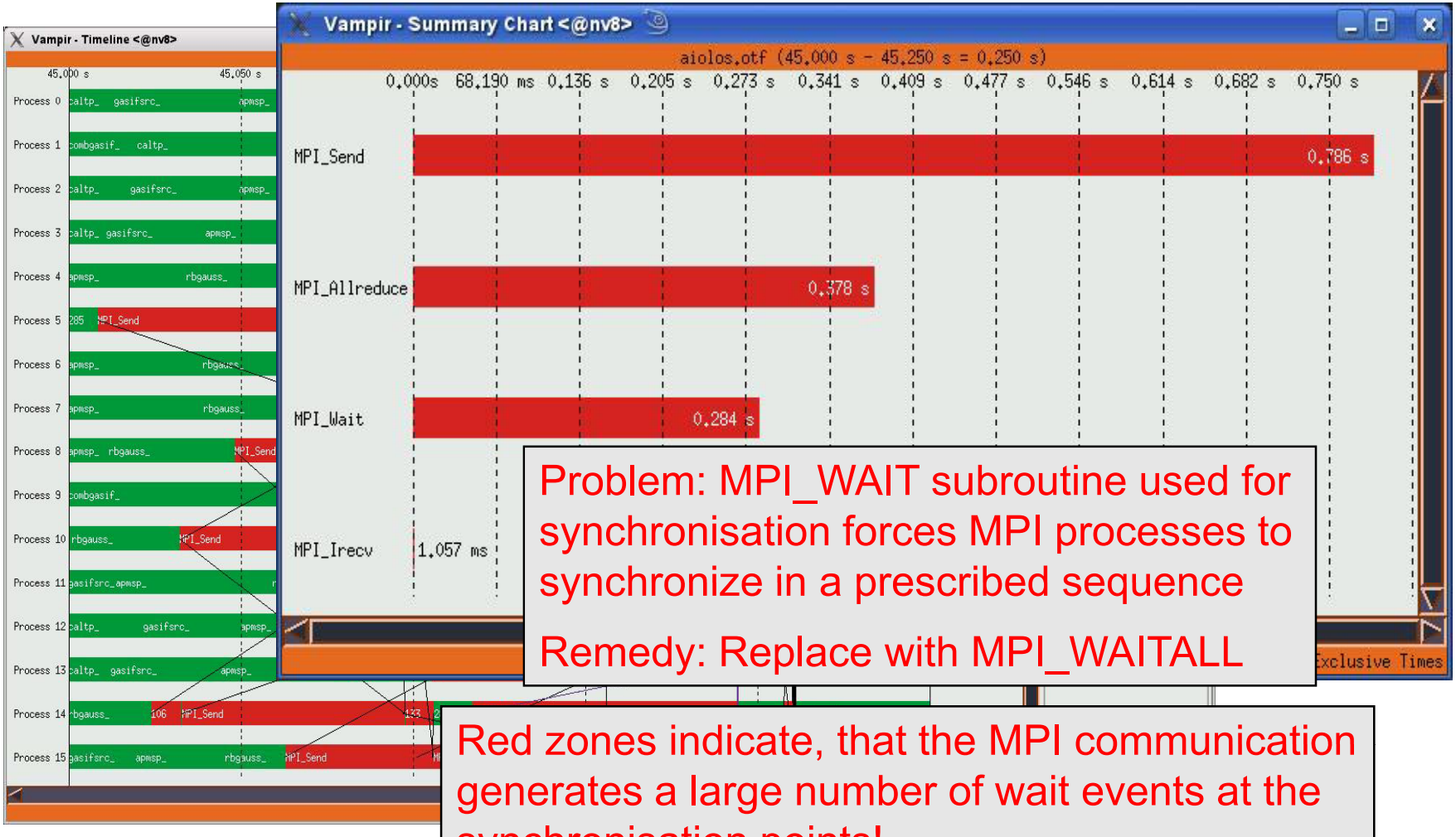
    ➡ Optimized execution on individual cores

- **High Level Performance Analysis of Hybrid Parallelism**
  - Investigate benefits of using hybrid (OpenMP and MPI) parallel execution within the node

    ➡ Optimized shared memory parallel execution within multi-core node

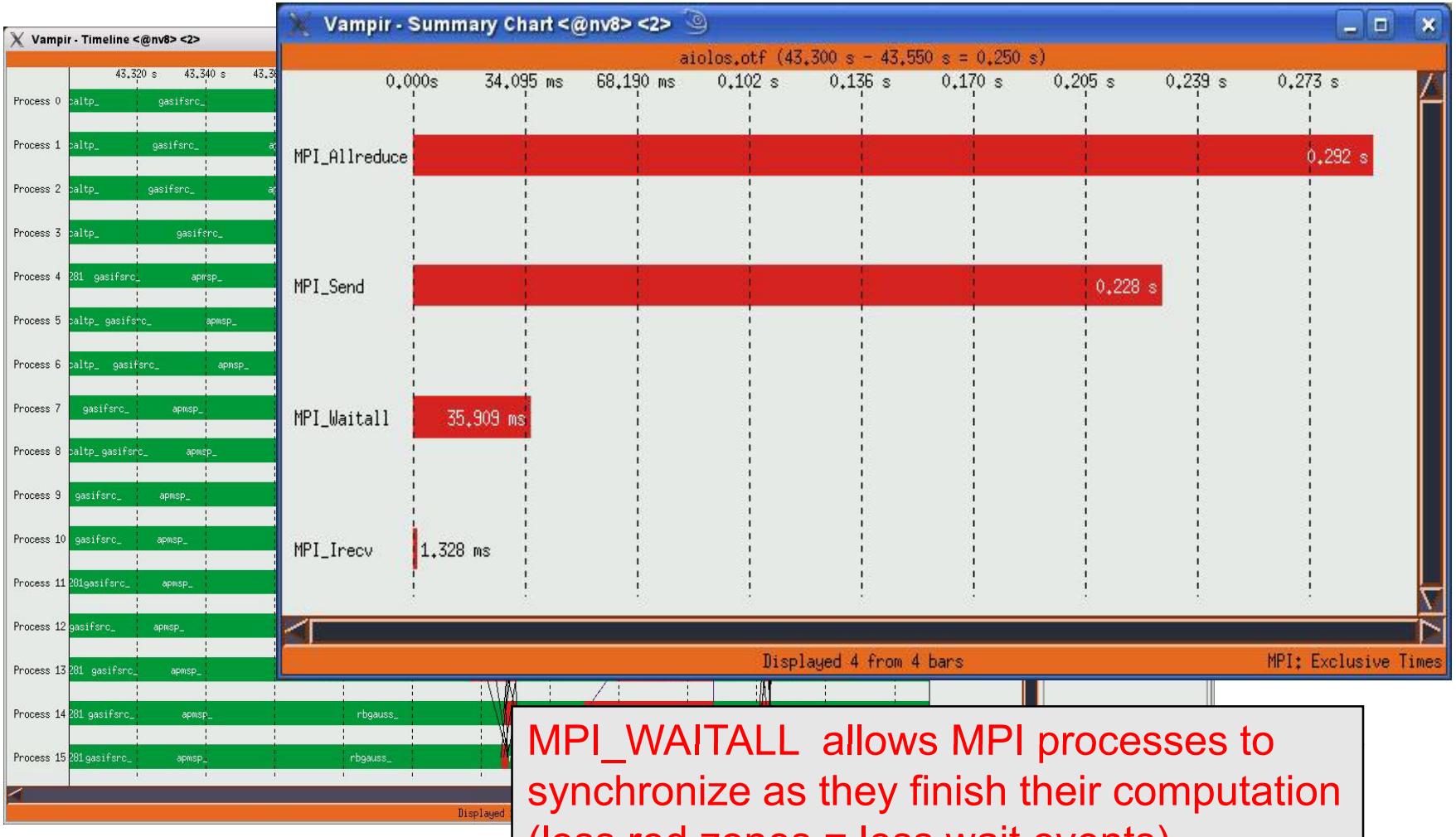
Example: VAMPIR Analysis of Original MPI-Communication

Portion of the code covering 0.25 s



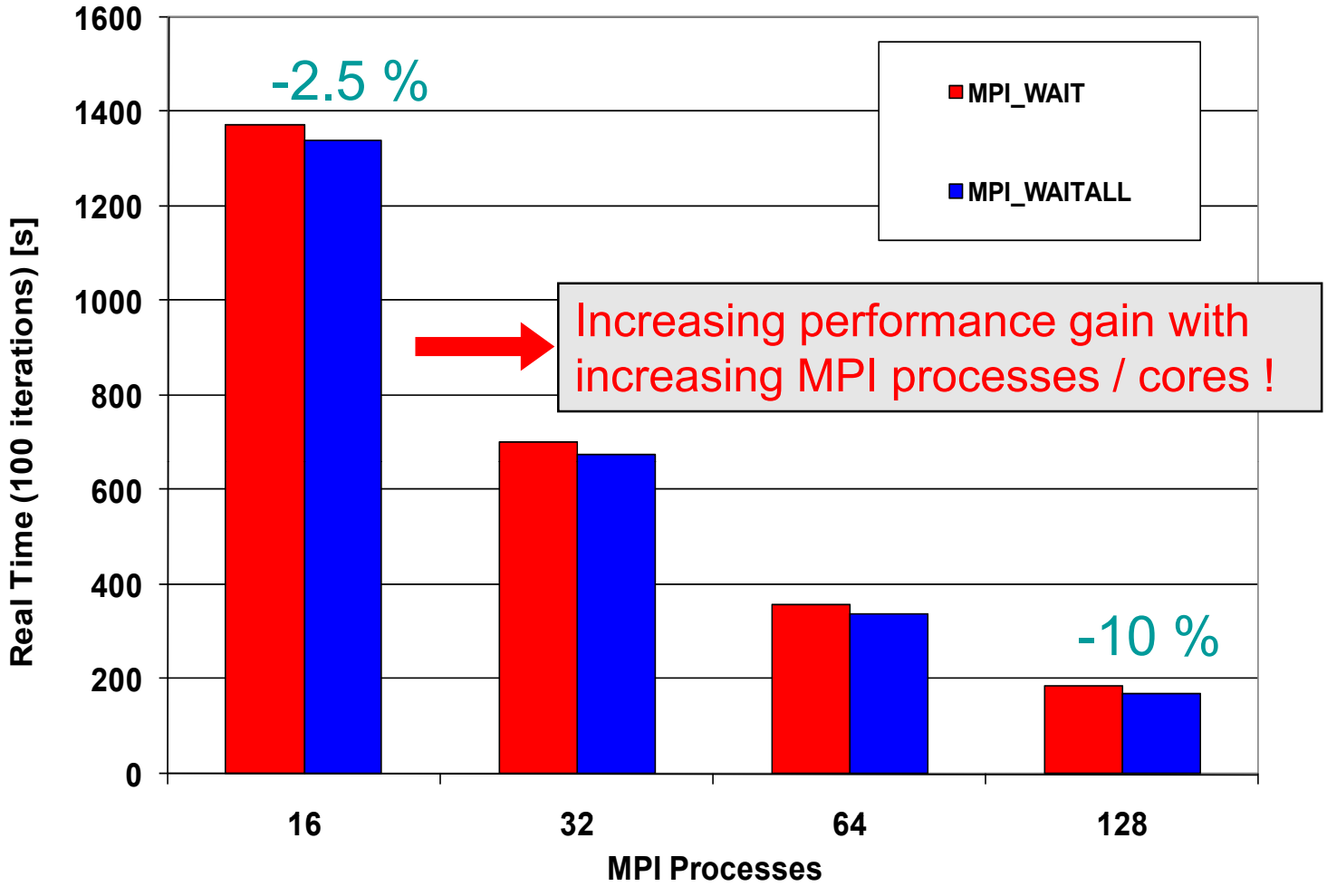
Example: VAMPIR Analysis of Modified MPI-Communication

Portion of the code covering the same 0.25 s

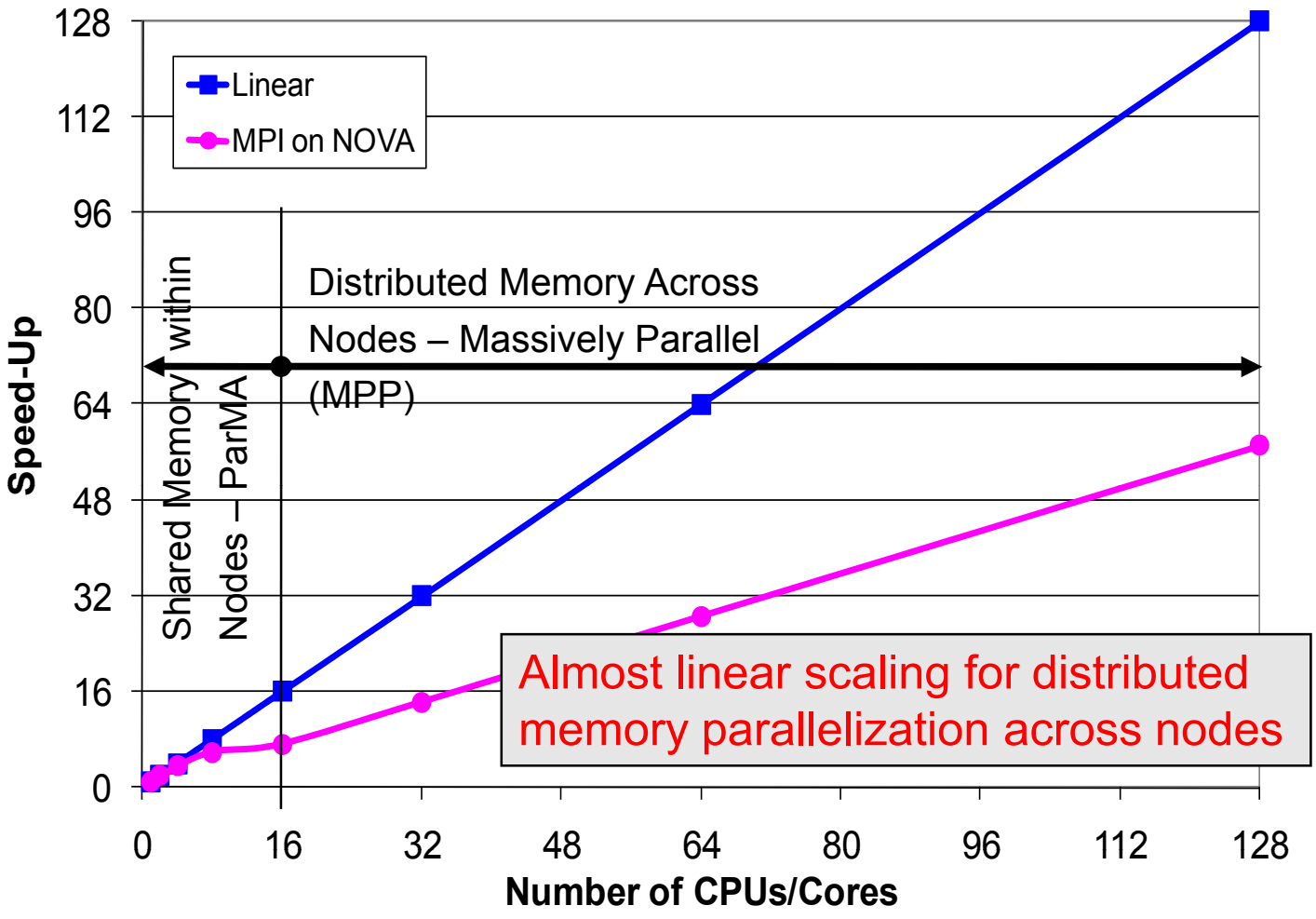


MPI_WAITALL allows MPI processes to synchronize as they finish their computation (less red zones = less wait events).

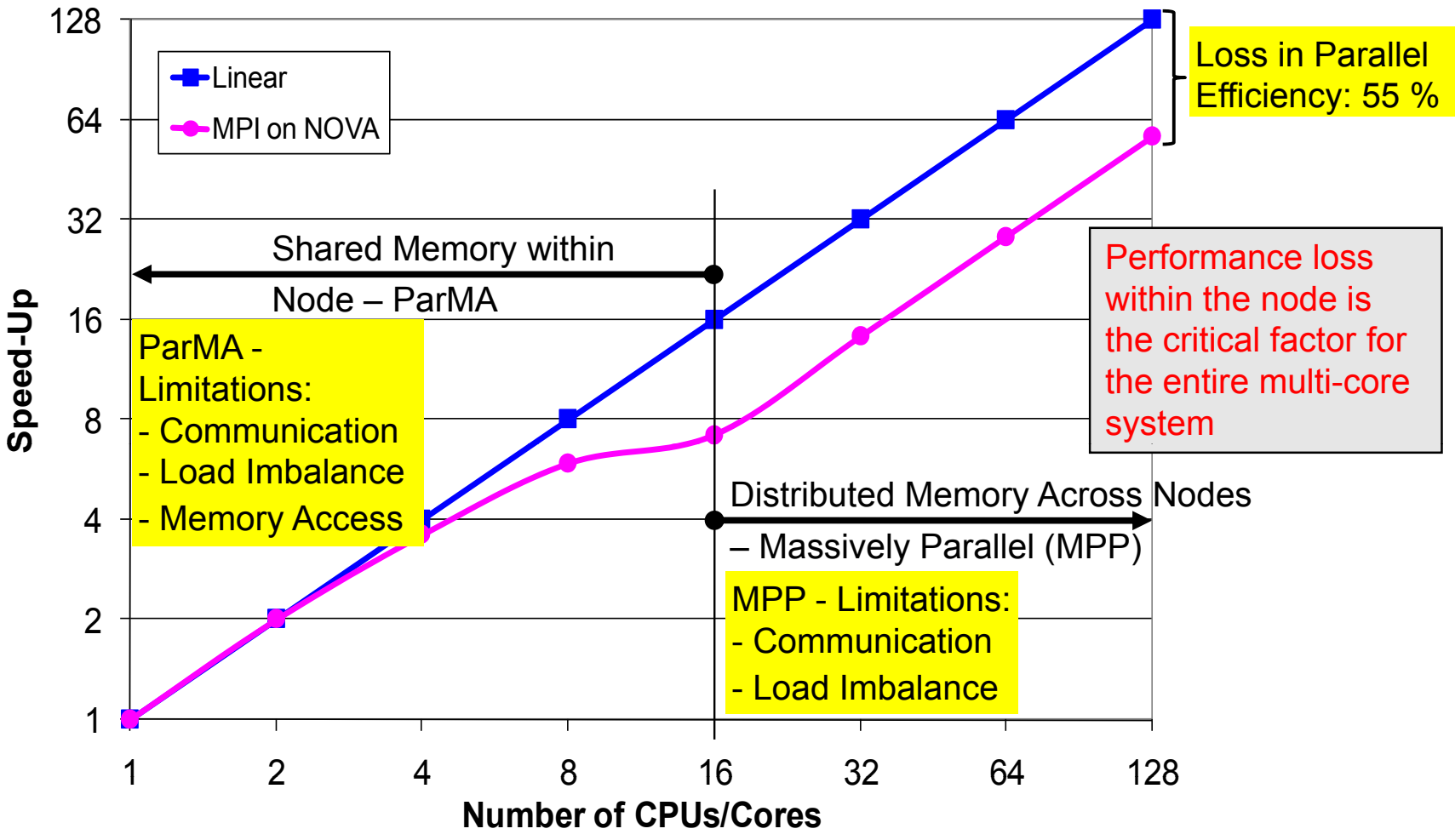
Performance improvement by exchange of MPI_WAIT with MPI_WAITALL



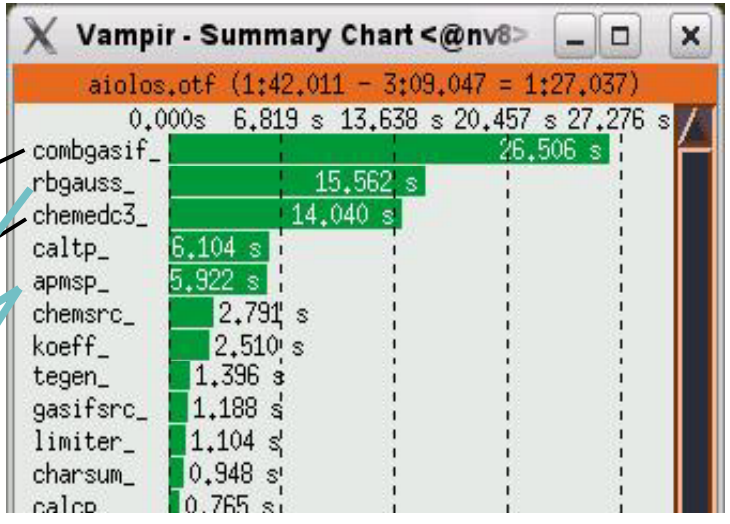
MPI Performance Analysis on Xeon-Cluster NOVA



A closer look to the Parallel Performance within the nodes

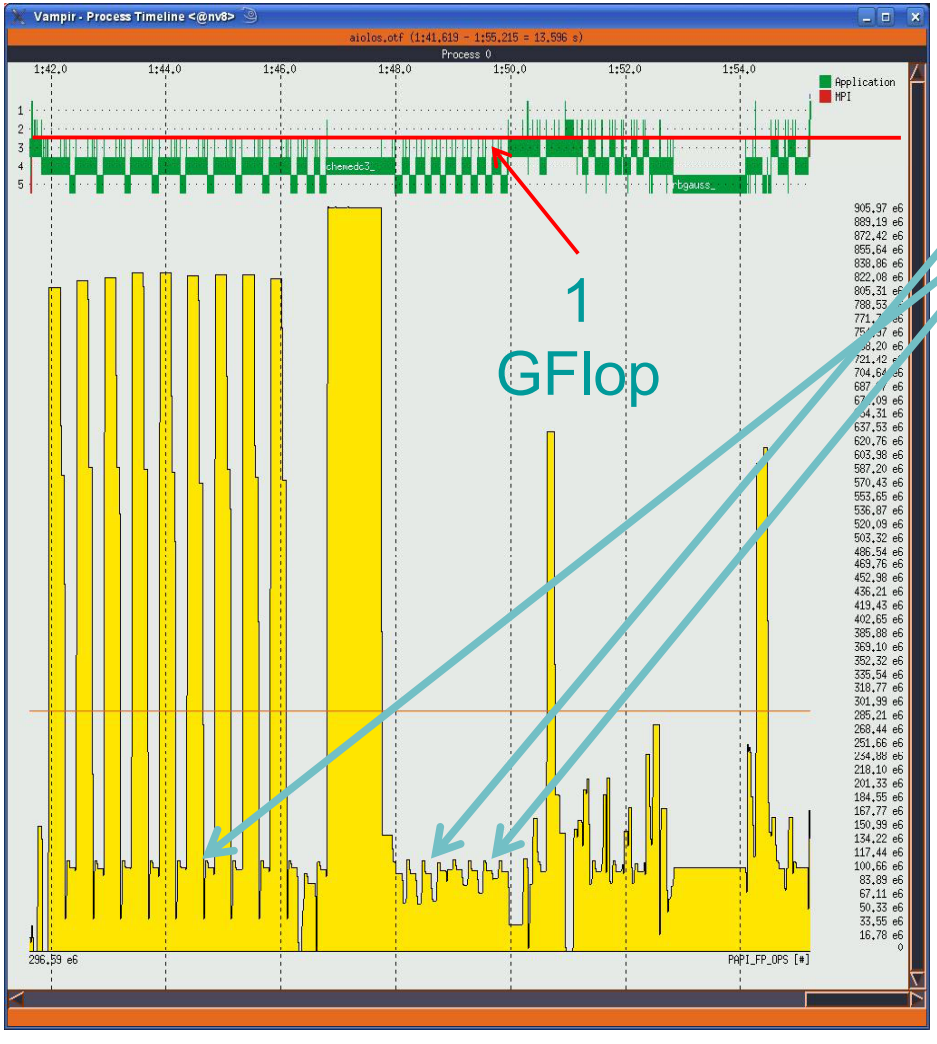


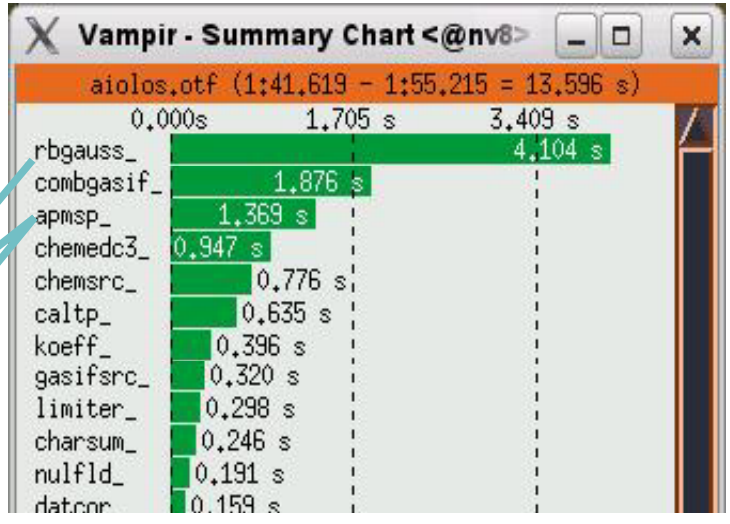
Analysis of subroutine Single Core performance using Flop counters



- combgasif approx. 930 Mflops
- chemedc3 approx. 970 Mflops
- rbgauss approx. 400 Mflops
- apmsp approx. 410 Mflops
  (about 6 % of total computing time)

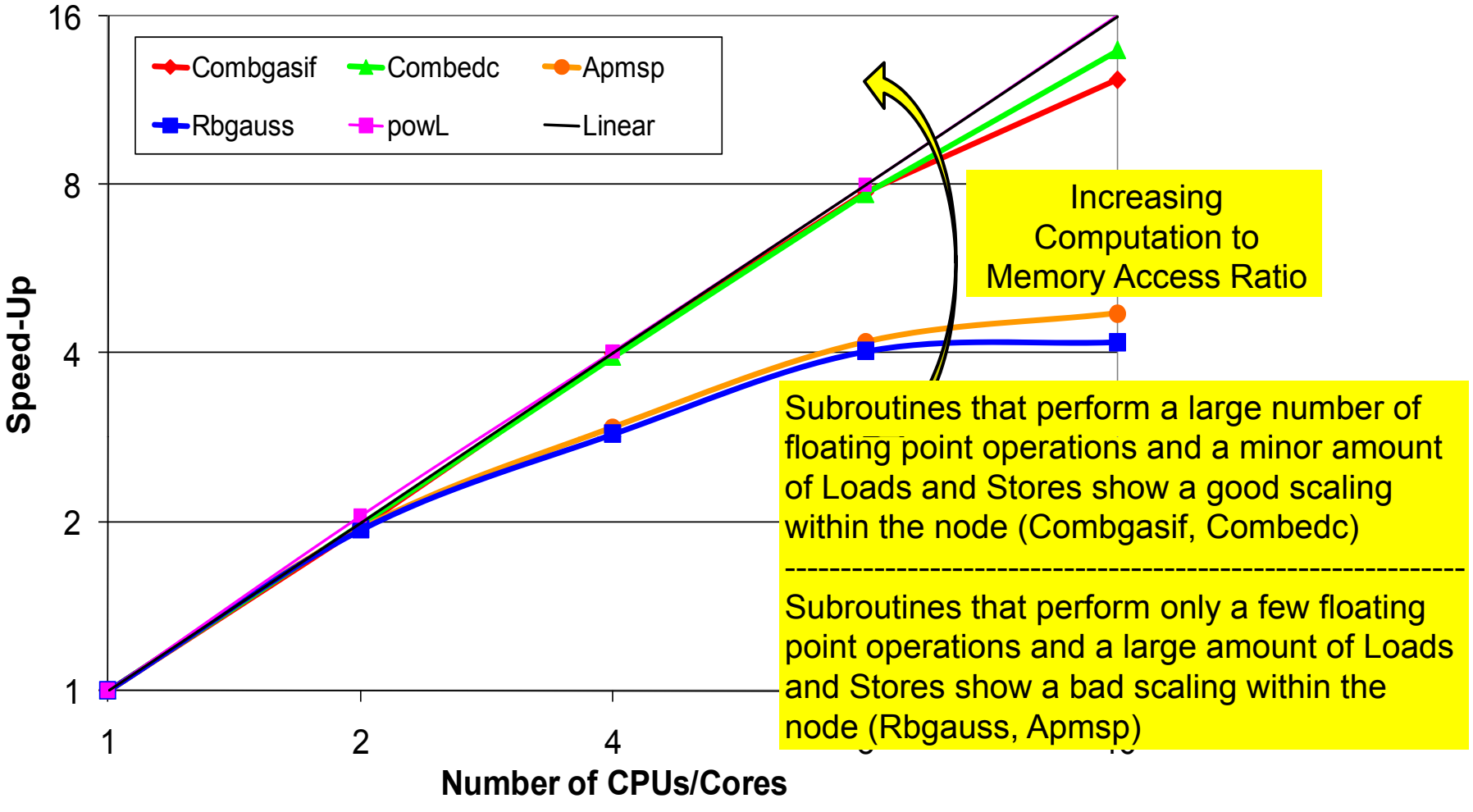
Analysis of subroutine Single Node (16 Cores) performance using Flop counters



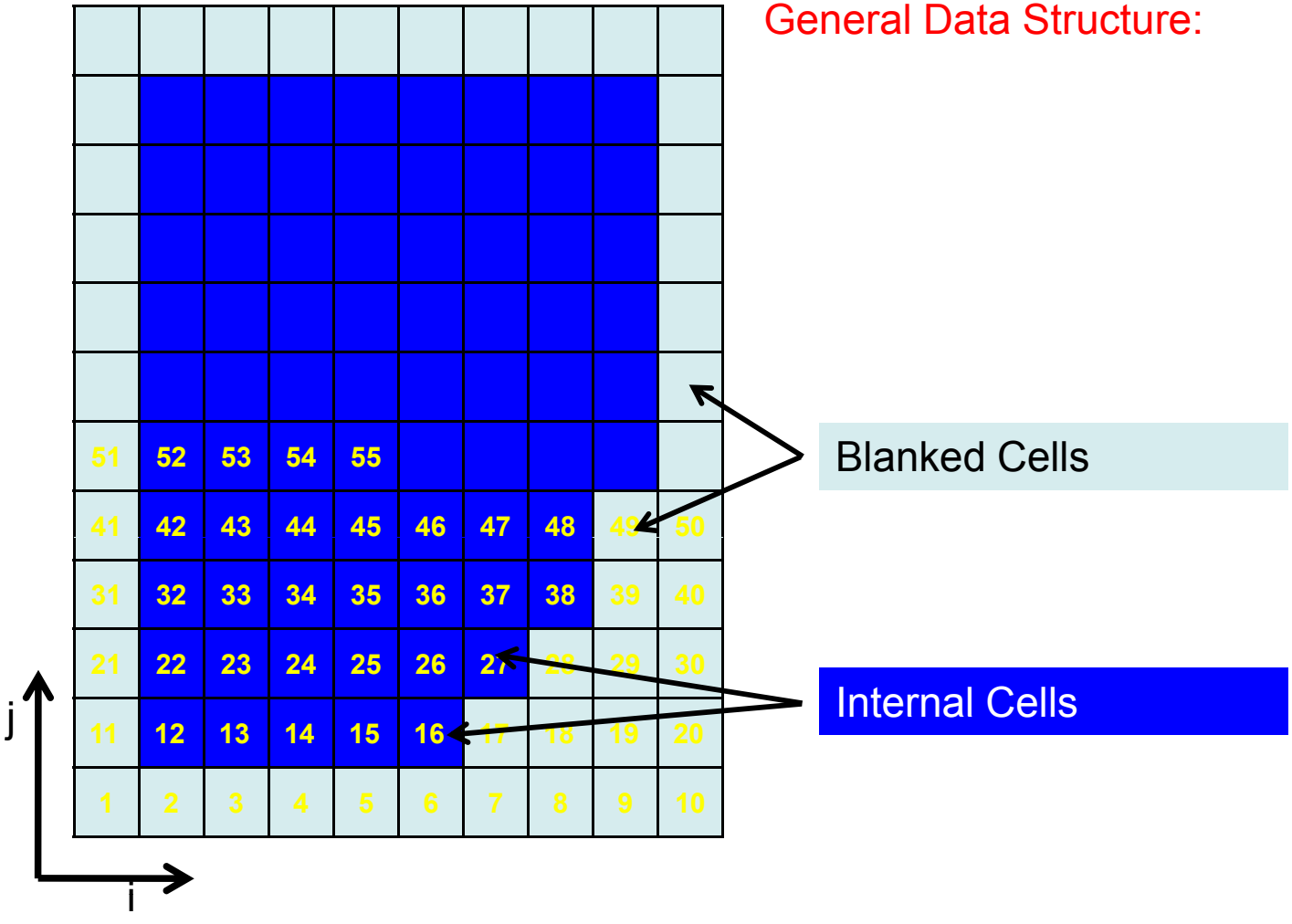


- combgasif approx. 820 Mflops
- chemedc3 approx. 910 Mflops
- rbgauss approx. 100 Mflops
- apmsp approx. 110 Mflops
  (about 10 % of total computing time)

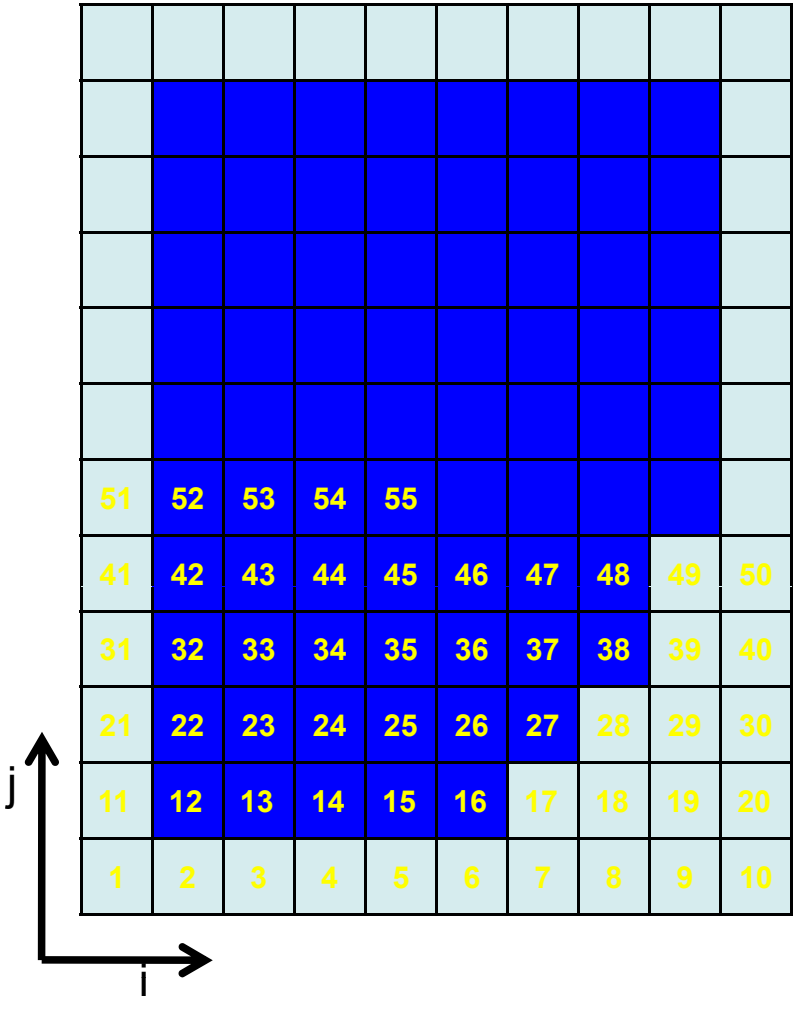
Parallel Single Node (16 Cores) performance on subroutine level



Data Structure of Rbgauss Subroutine



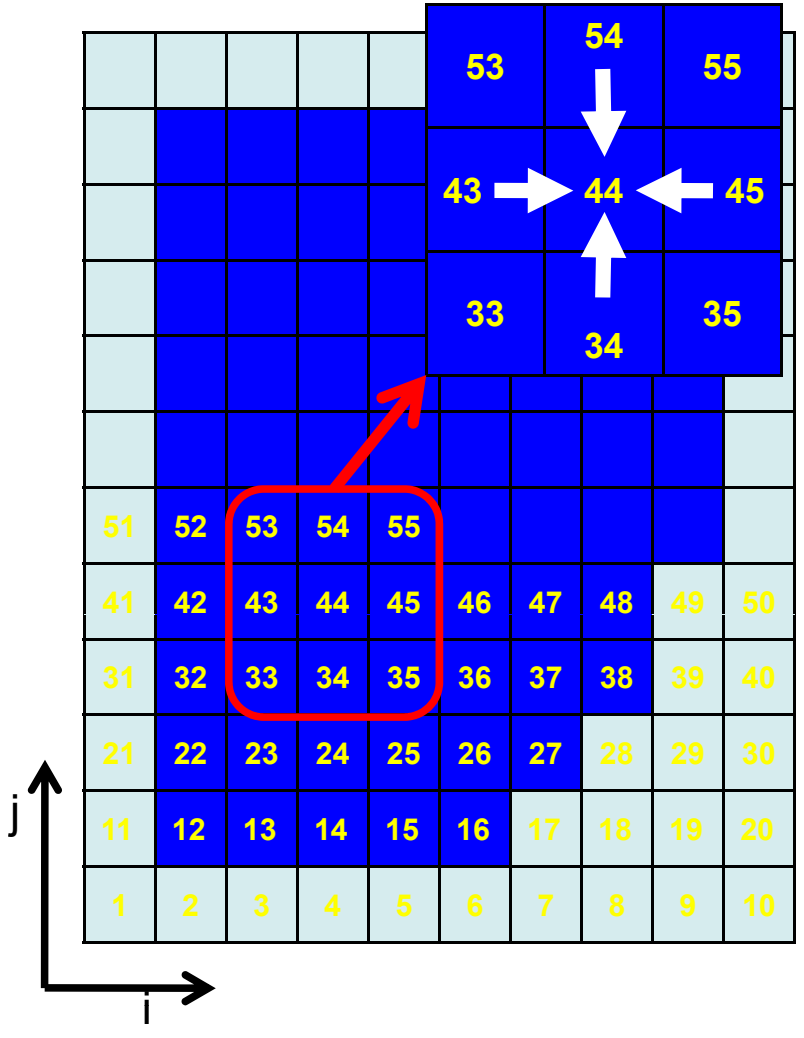
Principle of Gauss-Seidl Solver



Gauss-Seidl Solver for Transport Equations:

$$A_P \phi_P = \sum_{j=1}^{6} (A_j \phi_j) + S_\phi V$$

```
DO IDO=1,NINTERND
 INC = INDIN(IDO)
 ANS = AN(INC,1)*PHI(INC+1)      &
     + AN(INC,2)*PHI(INC-1)      &
     + AN(INC,3)*PHI(INC+INPD)   &
     + AN(INC,4)*PHI(INC-INPD)
     + SU(INC)
 PHI(INC) = ANS/AP(INC)
ENDDO
```



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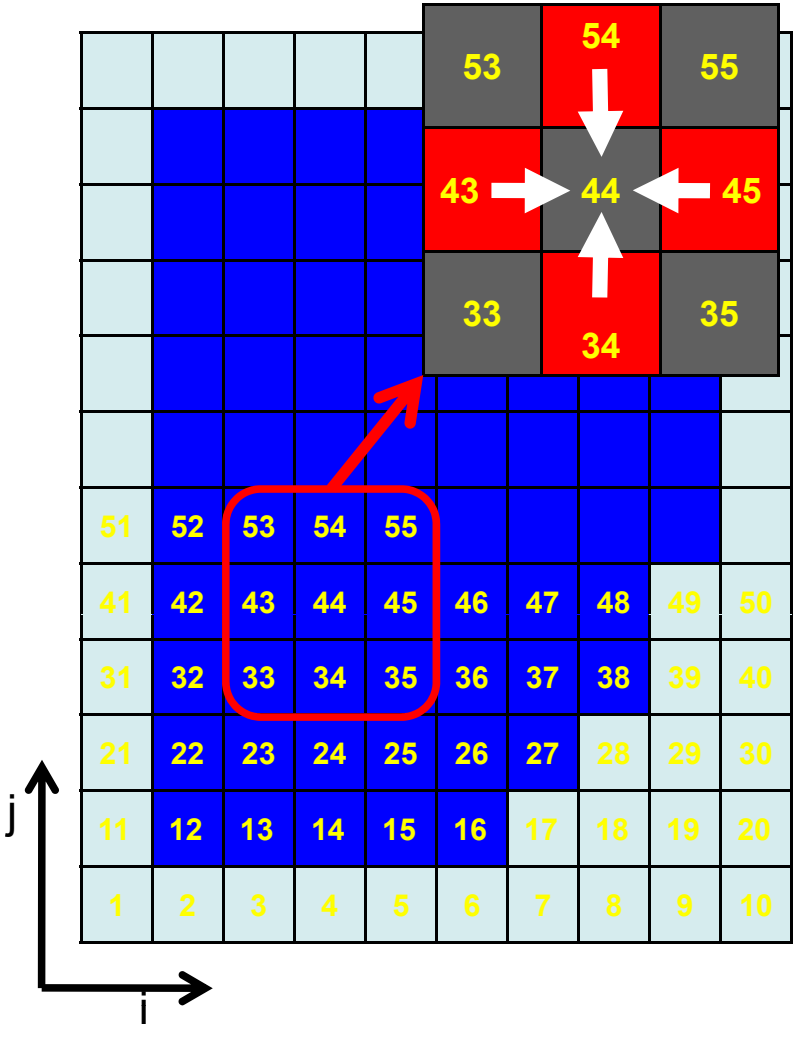
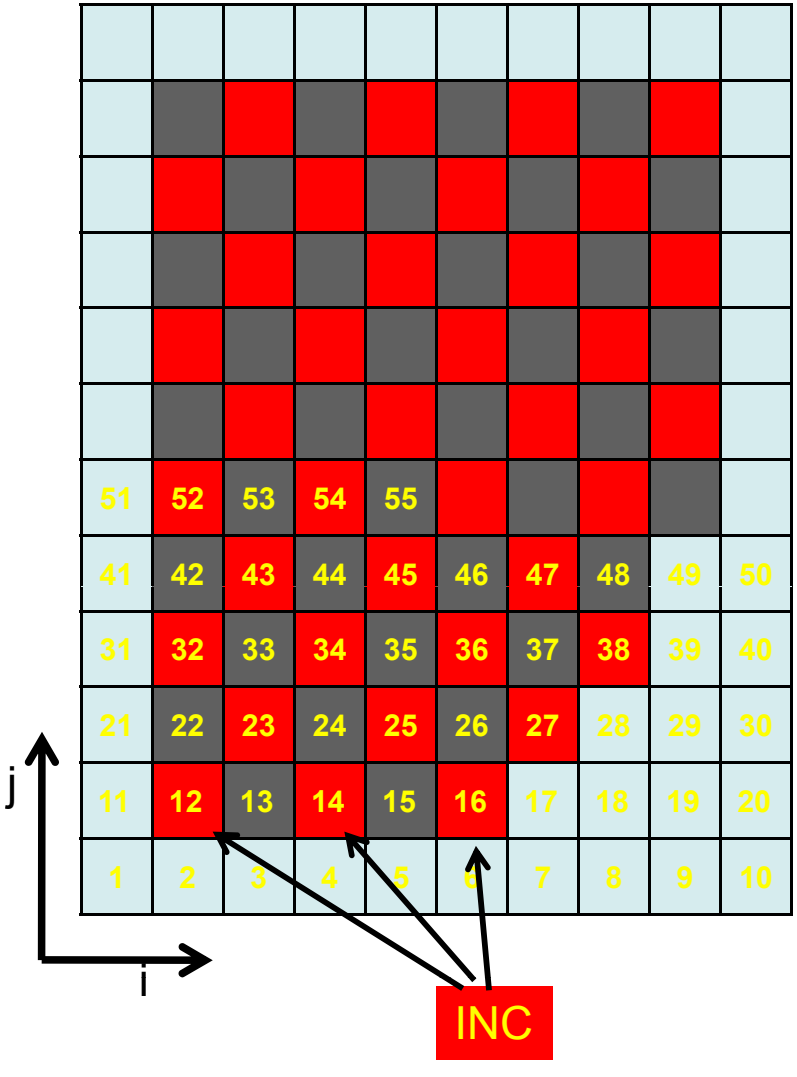
     + AN(INC,4)*PHI(INC-INPD)
     + SU(INC)
 PHI(INC) = ANS/AP(INC)
ENDDO
```

Structure of Rbgauss Subroutine



Gauss-Seidl Solver with Red-Black Ordering

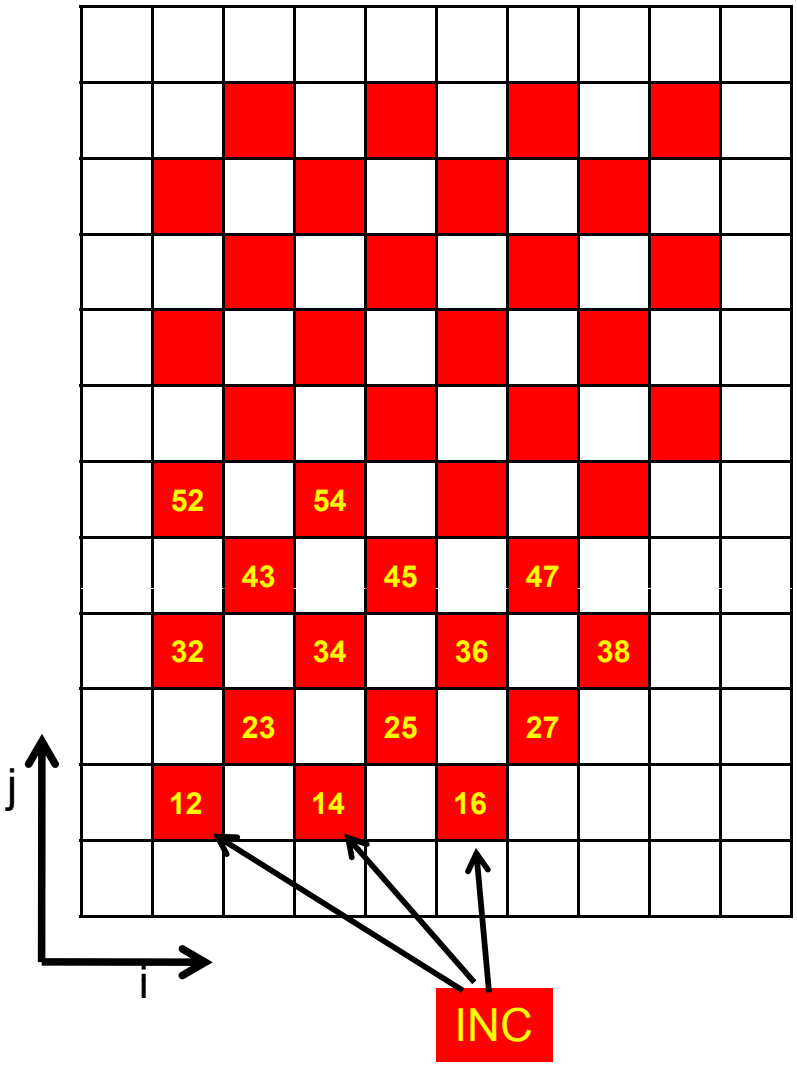
```
!$OMP PARALLEL DO PRIVATE(INC,ANS)
   DO IDO=1,NREDD
    INC = INDRED(IDO)
    ANS = AN(INC,1)*PHI(INC+1)      &
        + AN(INC,2)*PHI(INC-1)      &
        + AN(INC,3)*PHI(INC+INPD)   &
        + AN(INC,4)*PHI(INC-INPD)
        + SU(INC)
    PHI(INC) = ANS/AP(INC)
   ENDDO
!$OMP END PARALLEL DO
!$OMP PARALLEL DO PRIVATE(INC,ANS)
   DO IDO=1,NBLACKD
    INC = INDBLACK(IDO)
    ANS = AN(INC,1)*PHI(INC+1)      &
        + AN(INC,2)*PHI(INC-1)      &
        + AN(INC,3)*PHI(INC+INPD)   &
        + AN(INC,4)*PHI(INC-INPD)
        + SU(INC)
    PHI(INC) = ANS/AP(INC)
   ENDDO
!$OMP END PARALLEL DO
```



Red-Black Solver (Red Loop):

```
!!Red Loop of Red-Black-Solver
!$OMP PARALLEL DO PRIVATE(INC,ANS)
   DO IDO=1,NREDD
    INC = INDRED(IDO)
    ANS = AN(INC,1)*PHI(INC+1)      &
        + AN(INC,2)*PHI(INC-1)      &
        + AN(INC,3)*PHI(INC+INPD)   &
        + AN(INC,4)*PHI(INC-INPD)   &
        + SU(INC)
    PHI(INC) = ANS/AP(INC)
   ENDDO
!$OMP END PARALLEL DO
```

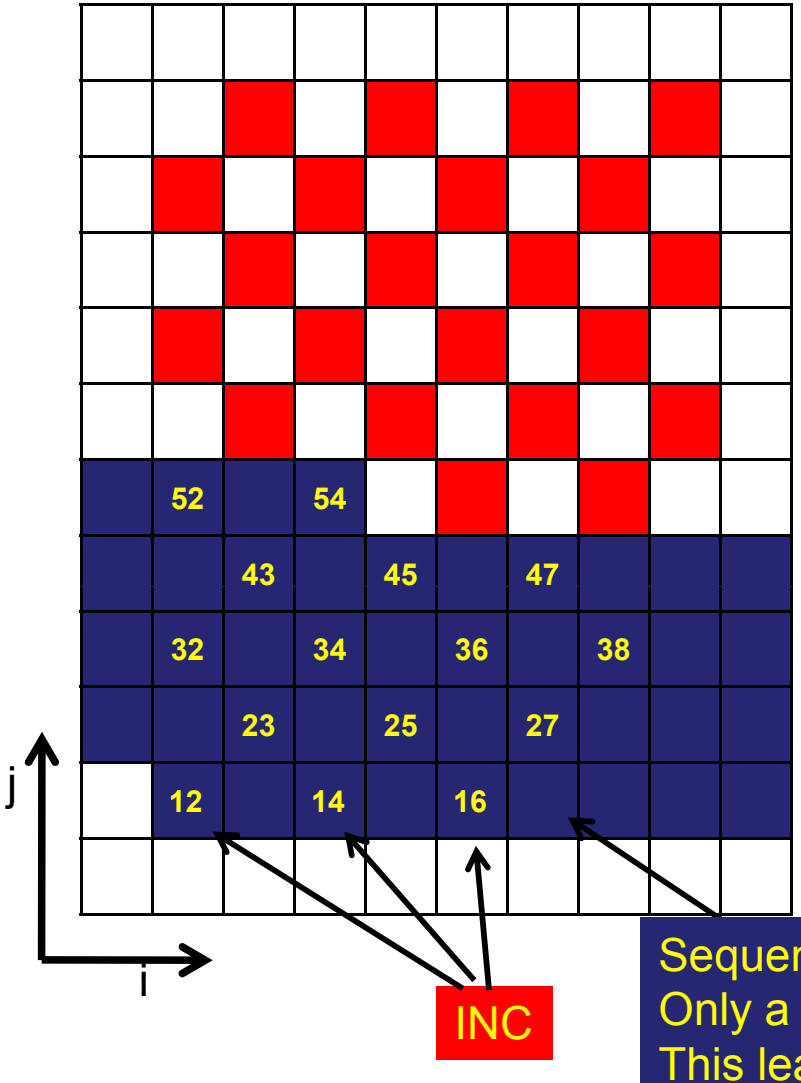
Problem of Rbgauss Subroutine



Only the Red AN / AP Elements are required

```
!!Red Loop of Red-Black-Solver
!$OMP PARALLEL DO PRIVATE(INC,ANS)
   DO IDO=1,NREDD
    INC = INDRED(IDO)
    ANS = AN(INC,1)*PHI(INC+1)      &
        + AN(INC,2)*PHI(INC-1)      &
        + AN(INC,3)*PHI(INC+INPD)   &
        + AN(INC,4)*PHI(INC-INPD)   &
        + SU(INC)
    PHI(INC) = ANS/AP(INC)
   ENDDO
!$OMP END PARALLEL DO
```

Problem of Rbgauss Subroutine



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        + AN(INC,2)*PHI(INC-1)      &
        + AN(INC,3)*PHI(INC+INPD)   &
        + AN(INC,4)*PHI(INC-INPD)   &
        + SU(INC)
    PHI(INC) = ANS/AP(INC)
   ENDDO
!$OMP END PARALLEL DO
```
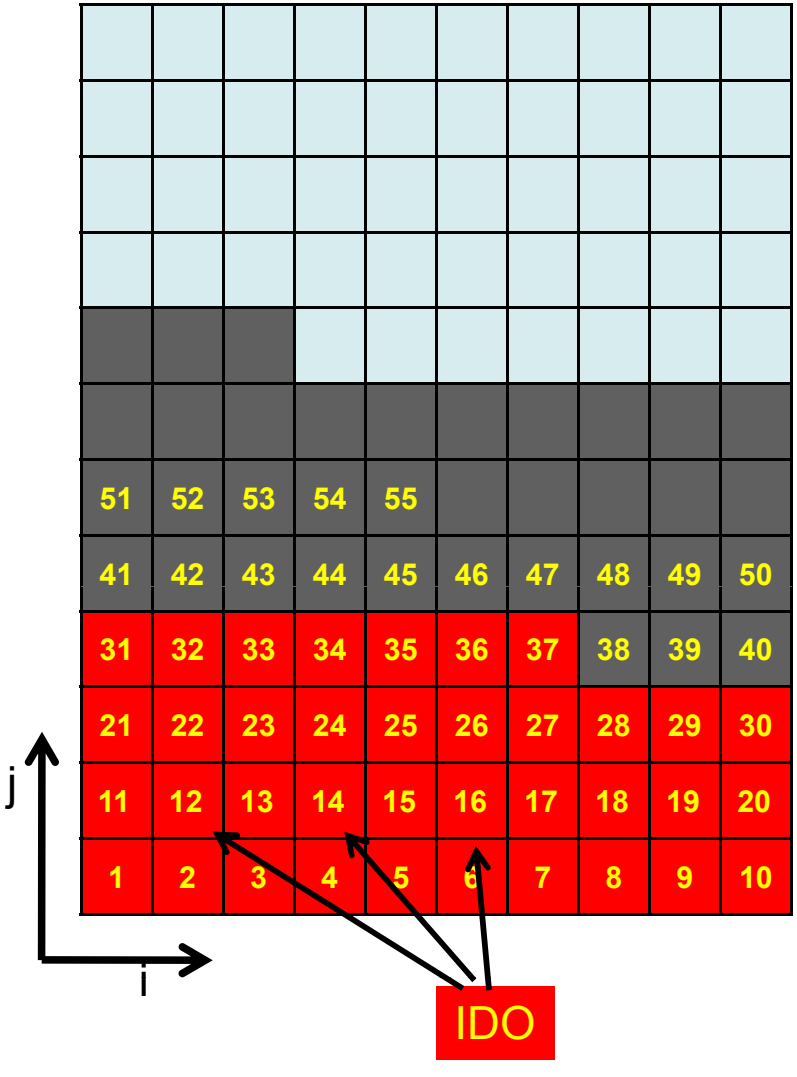

Sequential Cache Line:
Only a few elements loaded into cache are used !
This leads to a significant overhead in memory traffic !

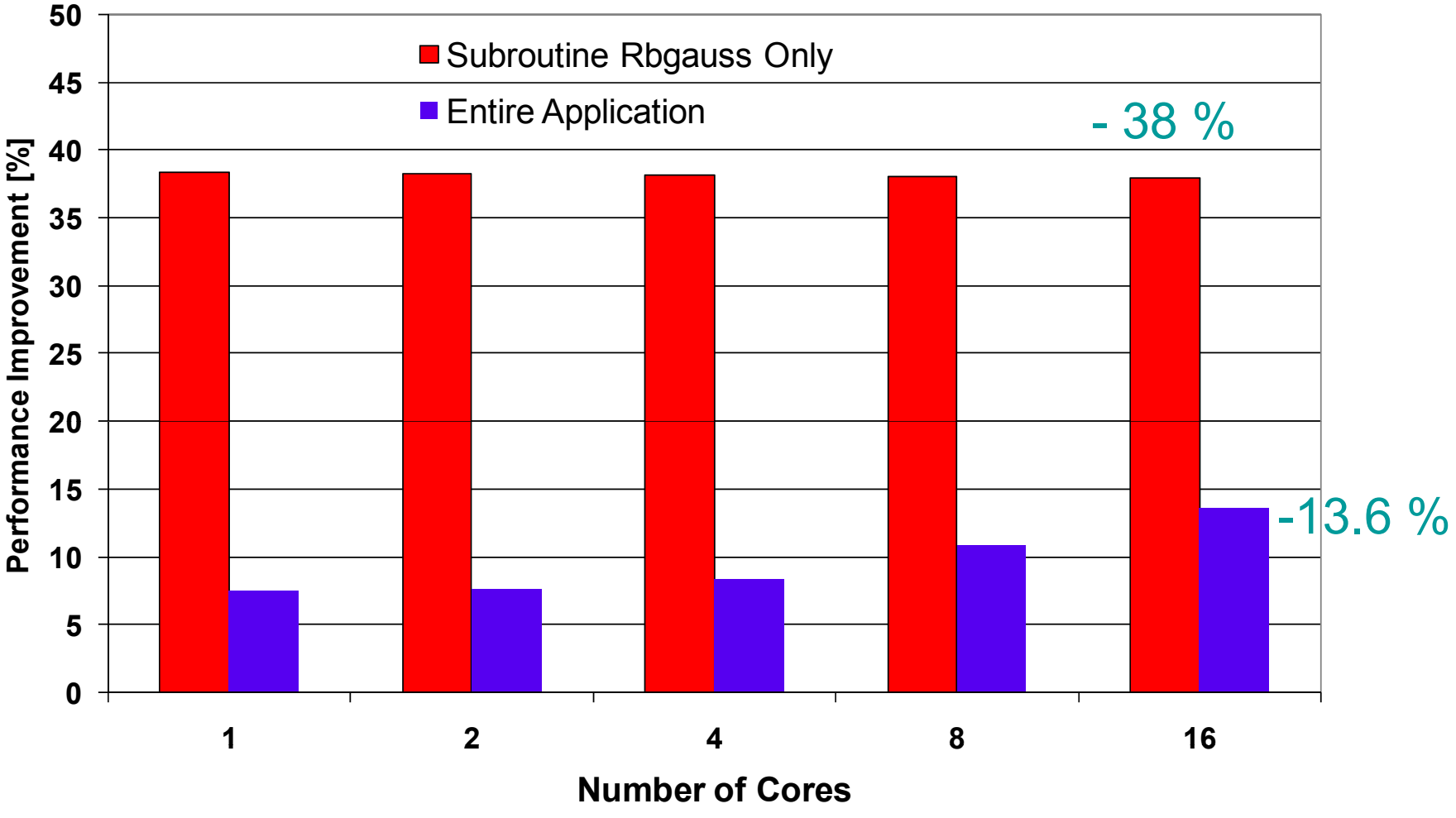
Improvement of Rbgauss Subroutine



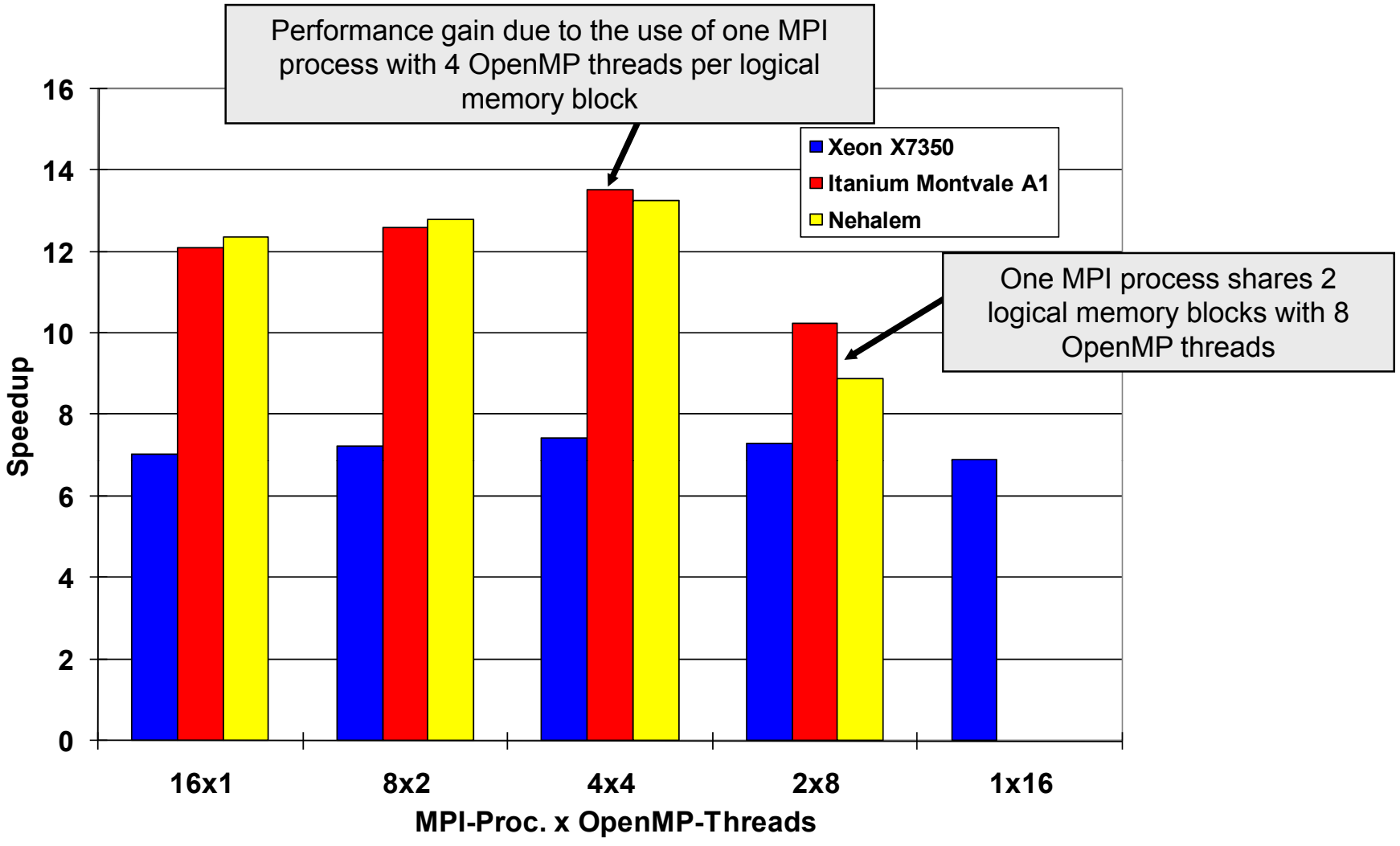
Reorientation of AN / AP Field:

```
!!Red Loop of Red-Black-Solver
!$OMP PARALLEL DO PRIVATE(INC,ANS)
   DO IDO=1,NREDD
    INC = INDRED(IDO)
    ANS = AN(IDO,1)*PHI(INC+1)      &
        + AN(IDO,2)*PHI(INC-1)      &
        + AN(IDO,3)*PHI(INC+INPD)   &
        + AN(IDO,4)*PHI(INC-INPD)   &
        + SU(INC)
    PHI(INC) = ANS/AP(IDO)
   ENDDO
!$OMP END PARALLEL DO
```

Performance improvement through Rbgauss restructuring



Maximizing the usage of the available memory bandwidth with a Hybrid (MPI & OpenMP) approach



Summary

- The ParMA tool chain allows a thorough analysis of the performance bottlenecks and the identification of the most promising measures for performance improvements.

- Even for a HPC-application like the 3D-Combustion Modelling Software RECOM-AIOLOS a performance gain of roughly 34% for the entire application has been achieved.