DEC code implementation and parallelization

Branislav Jansik

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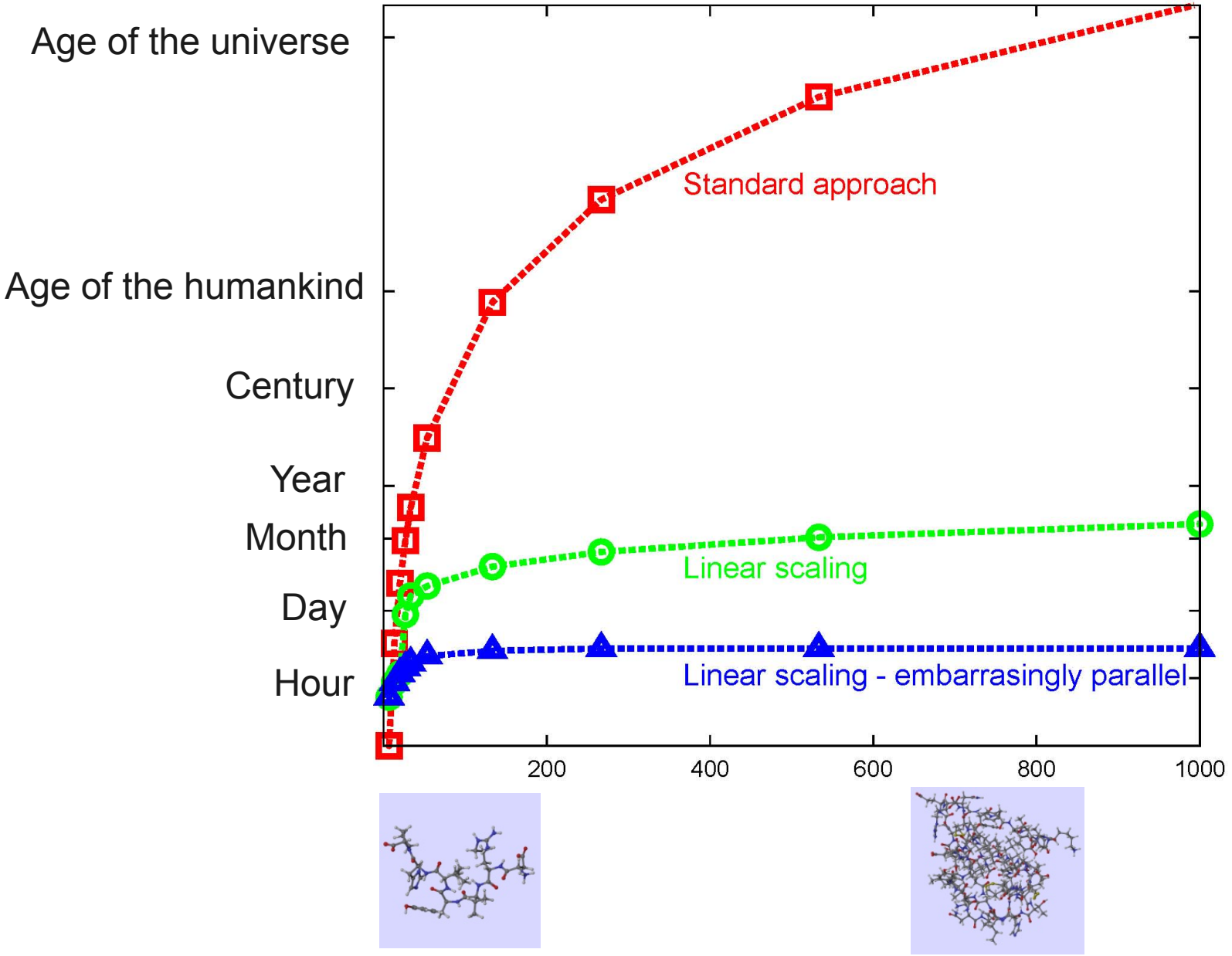
P. Ettenhuber and P. Jørgensen

Scaling in Coupled Cluster theory

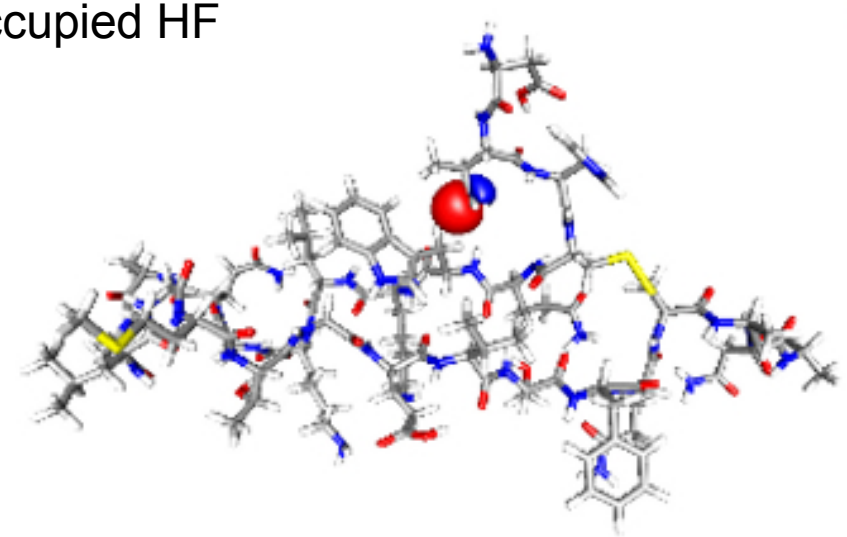


Fragment of Titin

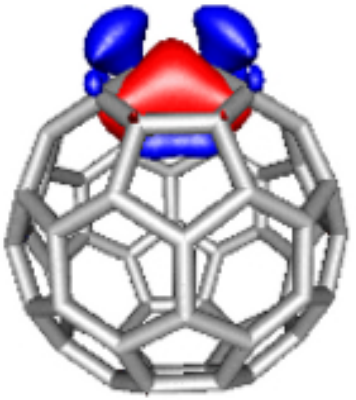
C_{60}

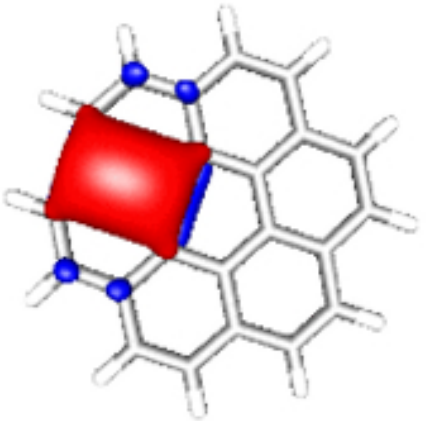
Super Benzene

Most delocalized
Occupied HF

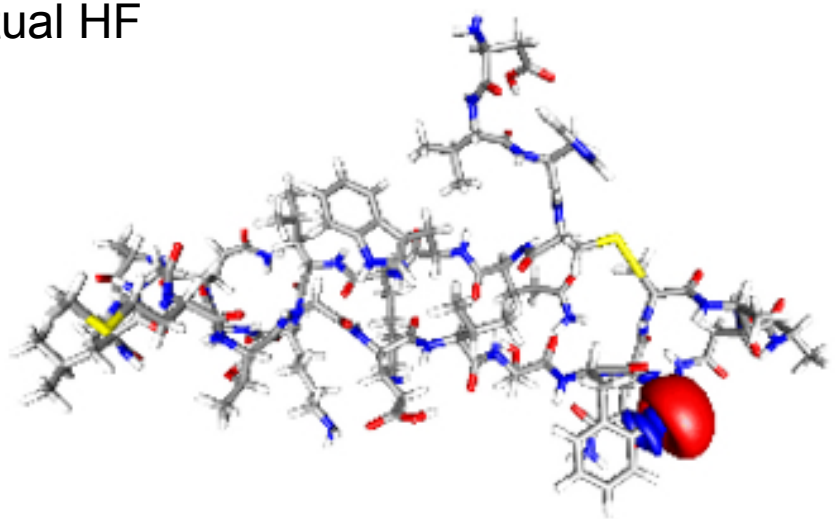


Occupied orbitals

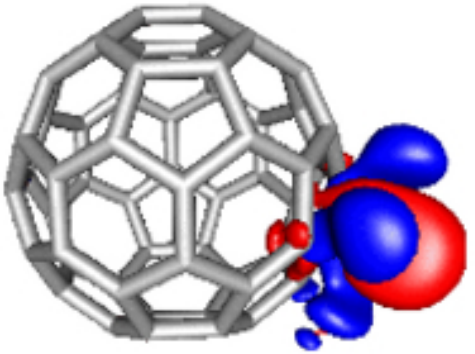


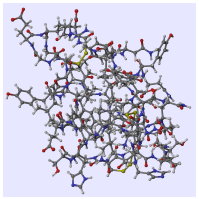


Most delocalized
Virtual HF



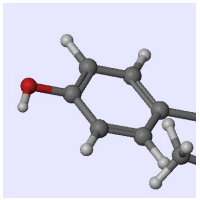
Virtual orbitals





Local HF orbitals

7604
bf



Atomic Fragment Optimization

P

Q

R

S

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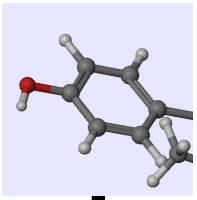
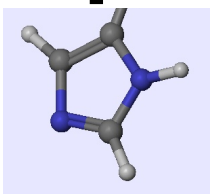
405





Pair fragment calculations

PQ

PR

QR

RS

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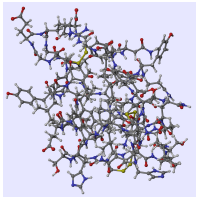
22484



Collection of results
For energy and density

PQ

Operation

- Compute batch of atomic integrals
- Transform to fragment canonical basis
- Solve equations
- Transform to local basis

Designed for

- Restrained memory requirements
- Easy hybrid parallelization

1: **for** $\tilde{\gamma}$ **do**
2: **for** $\tilde{\alpha}$ **do**
3: Calculate $g_{\tilde{\alpha}\tilde{\gamma}\beta\delta}$
4: $g_{\tilde{\alpha}\tilde{\gamma}\beta L} = \sum_{\delta} g_{\tilde{\alpha}\tilde{\gamma}\beta\delta} C_{\delta L}$
5: $g_{\tilde{\alpha}\tilde{\gamma}DL} = \sum_{\beta} g_{\tilde{\alpha}\tilde{\gamma}\beta L} C_{\beta D}$
6: $g_{\tilde{\alpha}\tilde{\gamma}bL} = \sum_{D} g_{\tilde{\alpha}\tilde{\gamma}DL} U_{bD}$
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8: $g_{cabL} += \sum_{\alpha\in\tilde{\alpha}} g_{\alpha abL} L_{\alpha c}$
9: $g_{\tilde{\alpha}\tilde{\gamma}Dj} = \sum_{L} g_{\tilde{\alpha}\tilde{\gamma}DL} U_{jL}$
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12: $g_{\tilde{\alpha}KDL} = \sum_{\gamma\in\tilde{\gamma}} g_{\tilde{\alpha}\gamma DL} C_{\gamma K}$
13: **for** $\tilde{C}$ **do**
14: $g_{\tilde{C}KDL} = \sum_{\alpha\in\tilde{\alpha}} g_{\tilde{\alpha}KDL} C_{\alpha\tilde{C}}$
15: $t_{\tilde{C}KDL} = g_{\tilde{C}KDL} / \varepsilon^{\tilde{C}D\prime}_{KL}$
16: $X_{\tilde{C}iDL} = \sum_{K} X_{\tilde{C}KDL} U_{iK}$
17: $X_{CiDj} += \sum_{L} X_{\tilde{C}iDL} U_{jL}$
18: $X_{\tilde{C}KbL} = \sum_{D} X_{\tilde{C}KDL} U_{bD}$
19: $X_{aKbL} += \sum_{C\in\tilde{C}} X_{CKbL} U_{aC}$
20: **end for** $\tilde{C}$
21: **end for** $\tilde{\alpha}$
22: **end for** $\tilde{\gamma}$
23: $X_{Cidj} = \sum_{D} X_{CiDj} U_{dD}$
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28: $g_{acbk} = g_{cabk} = \sum_{L} g_{cabL} U_{kL}$

PQ

DGEMM

1: **for** $\tilde{\gamma}$ **do**
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PQ

OMP

DGEMM (OMP)

OMP

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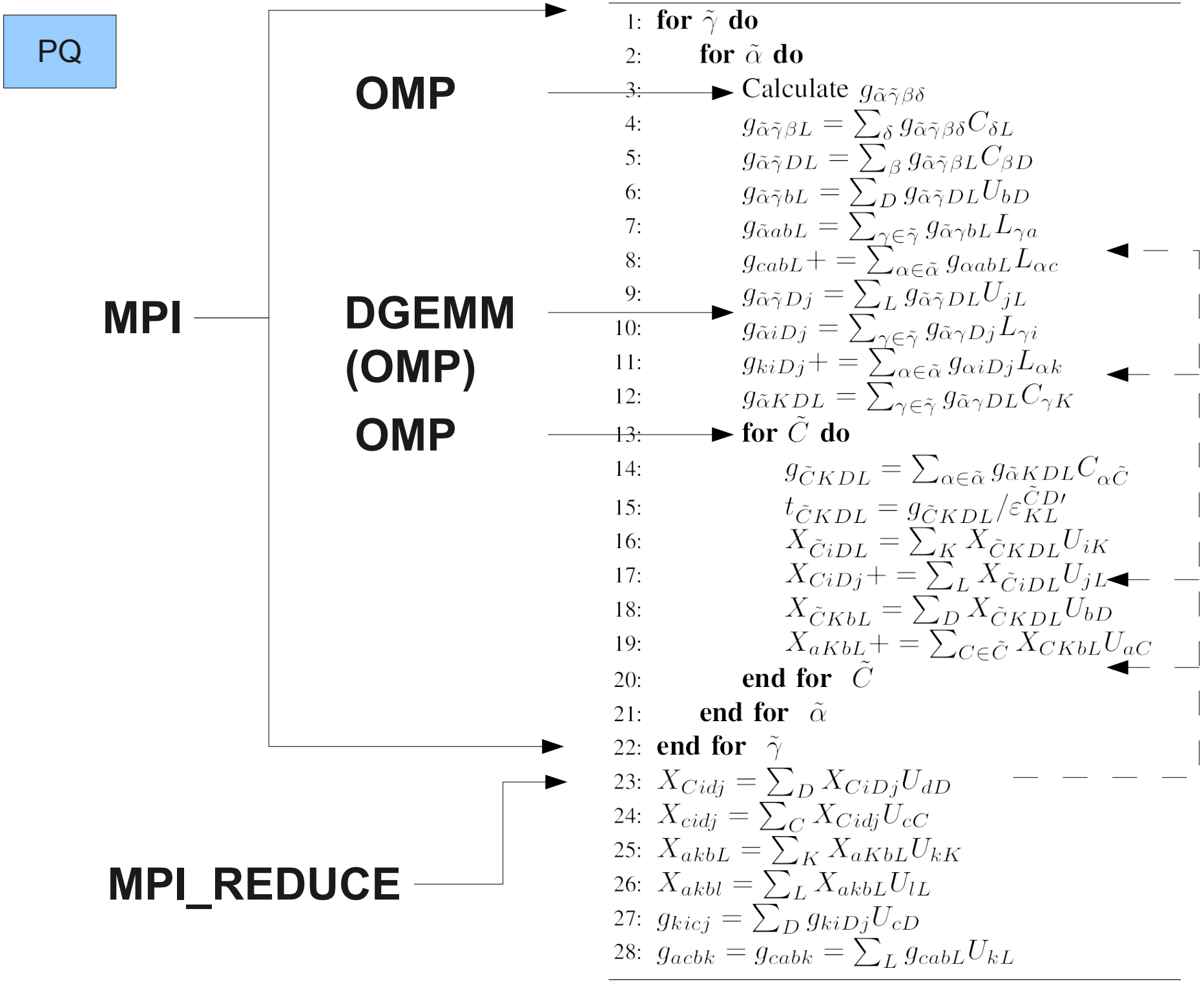
PQ
OMP
MPI
DGEMM
(OMP)
OMP
MPI_REDUCE
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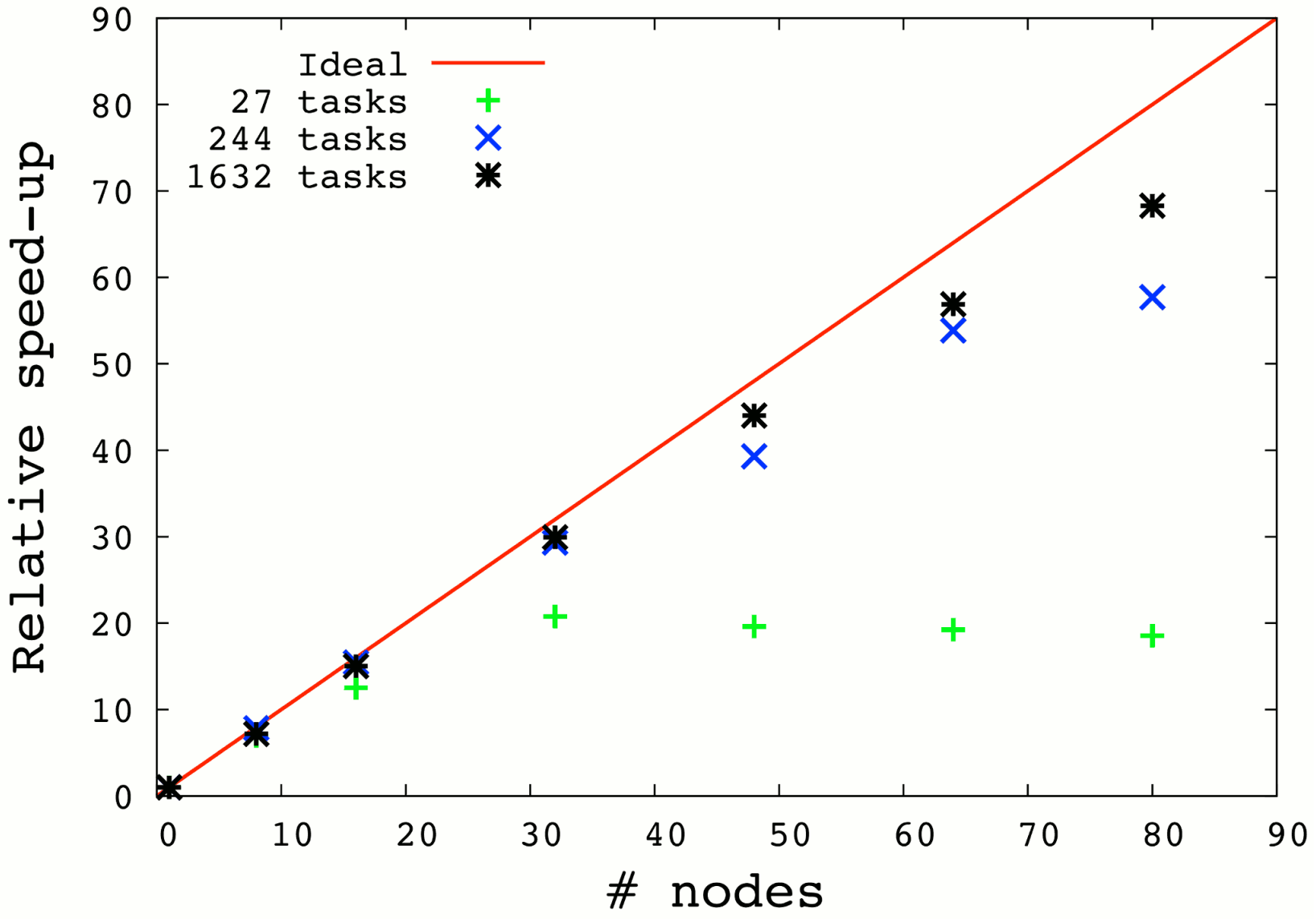
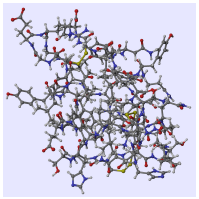
PQ

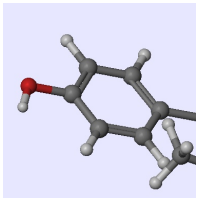
MPI parallel performance





Local HF orbitals

7604
bf



Atomic Fragment Optimization

P

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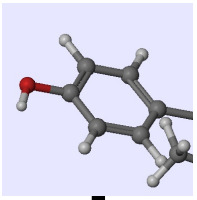

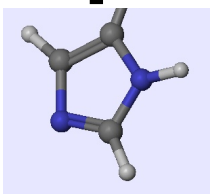

Pair fragment calculations

PQ

PR

QR

RS

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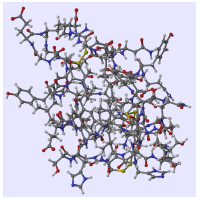
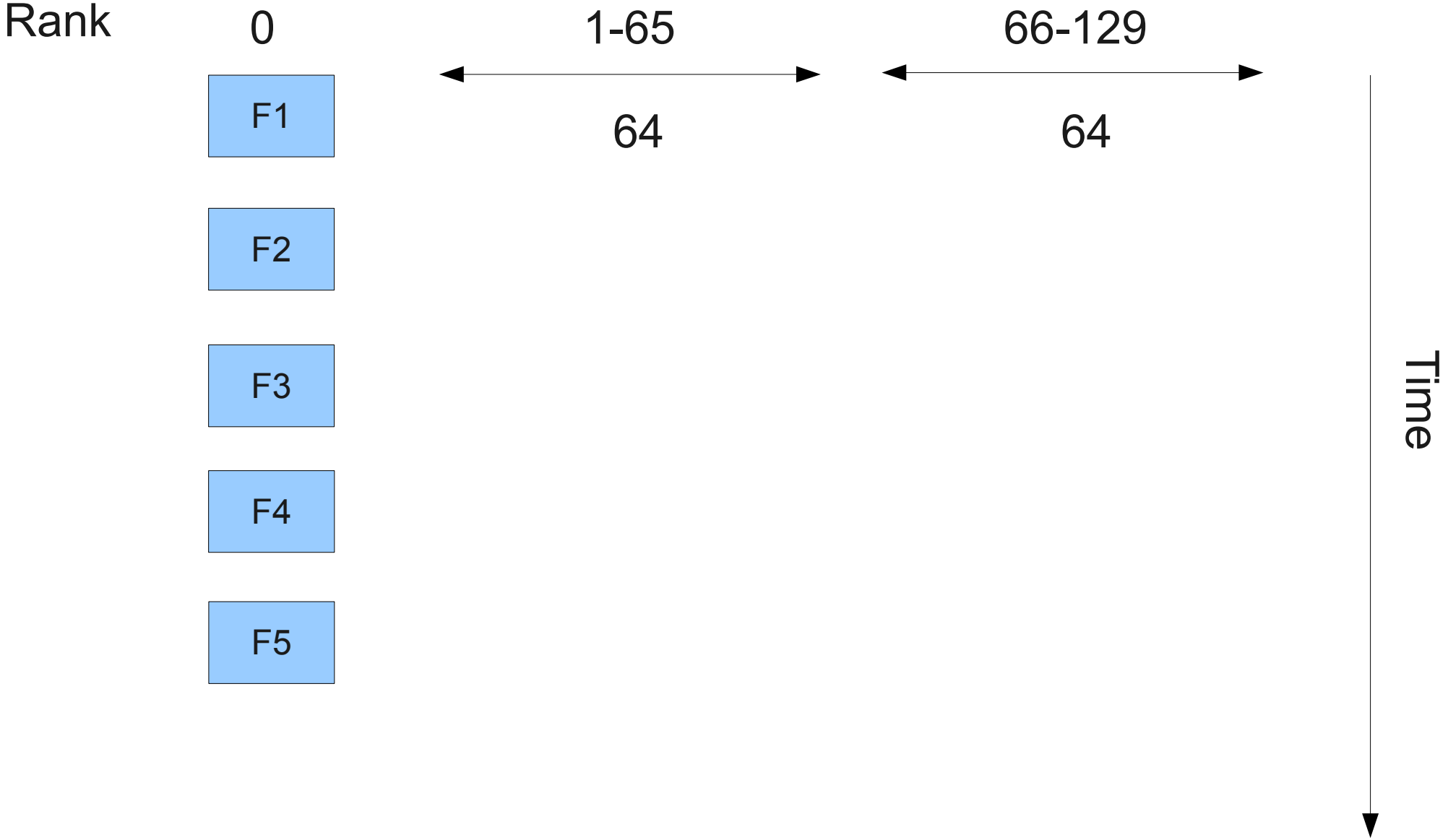
22484

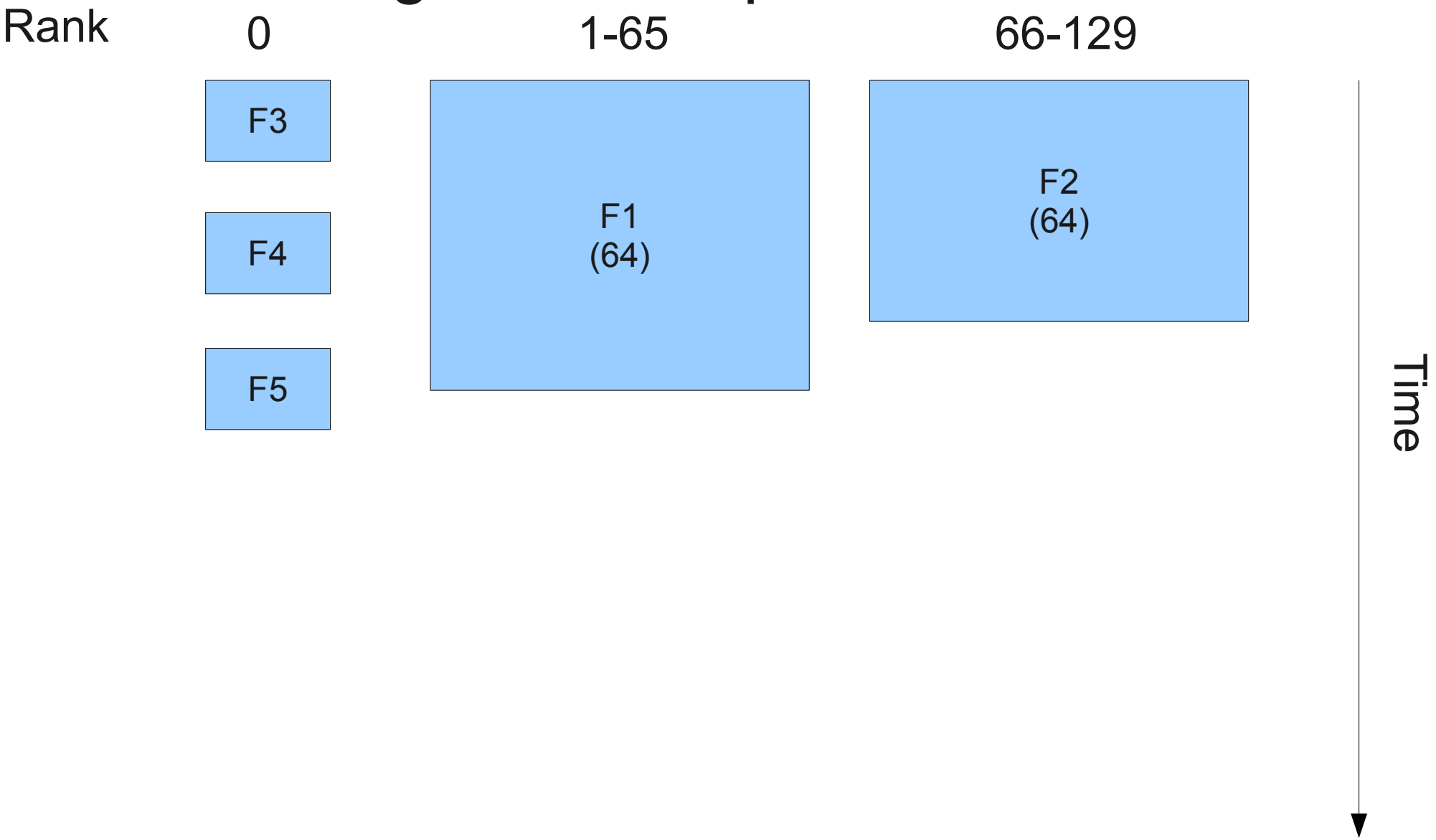


Collection of results
For energy and density

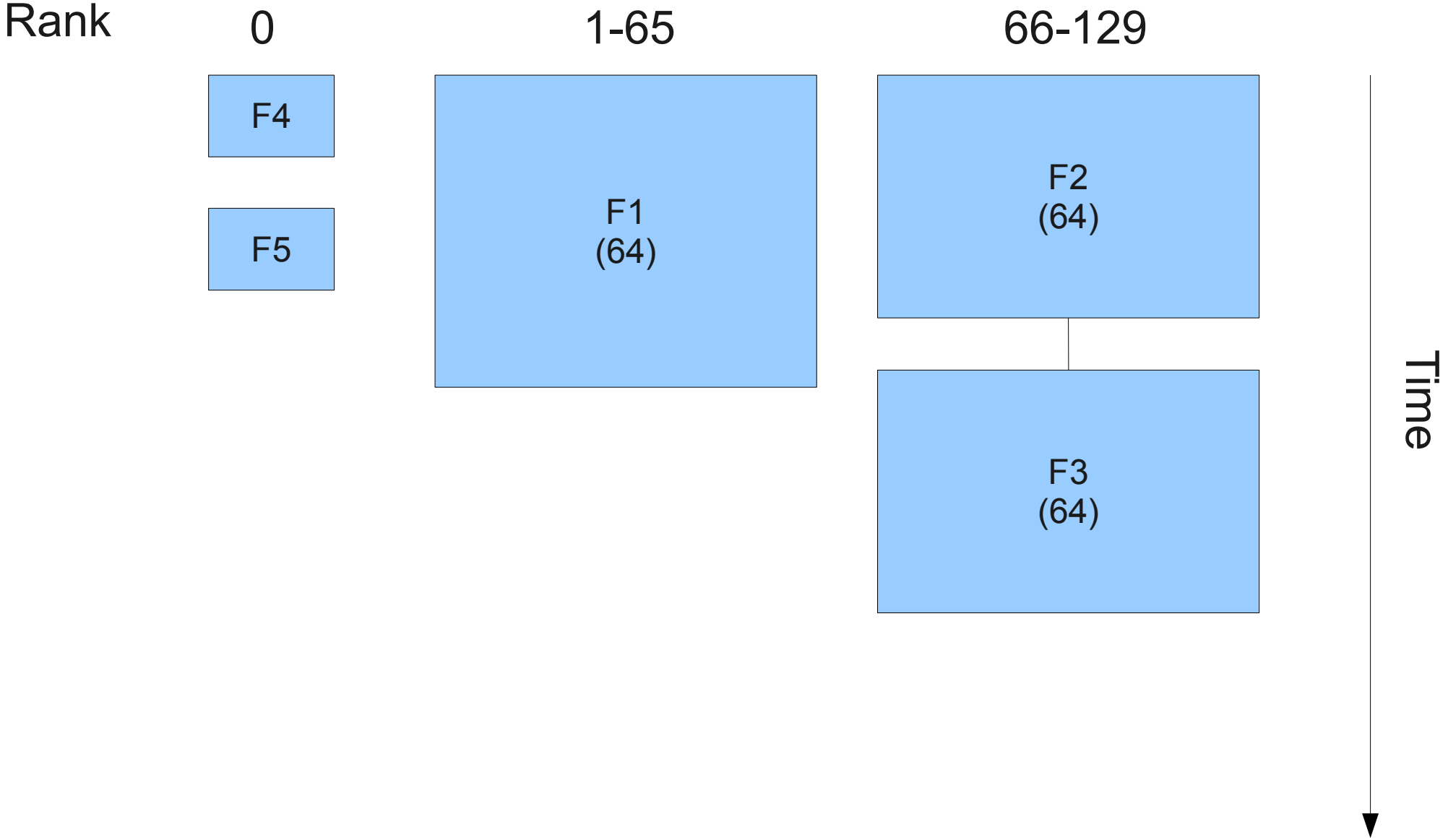
Pair fragment MPI parallelization



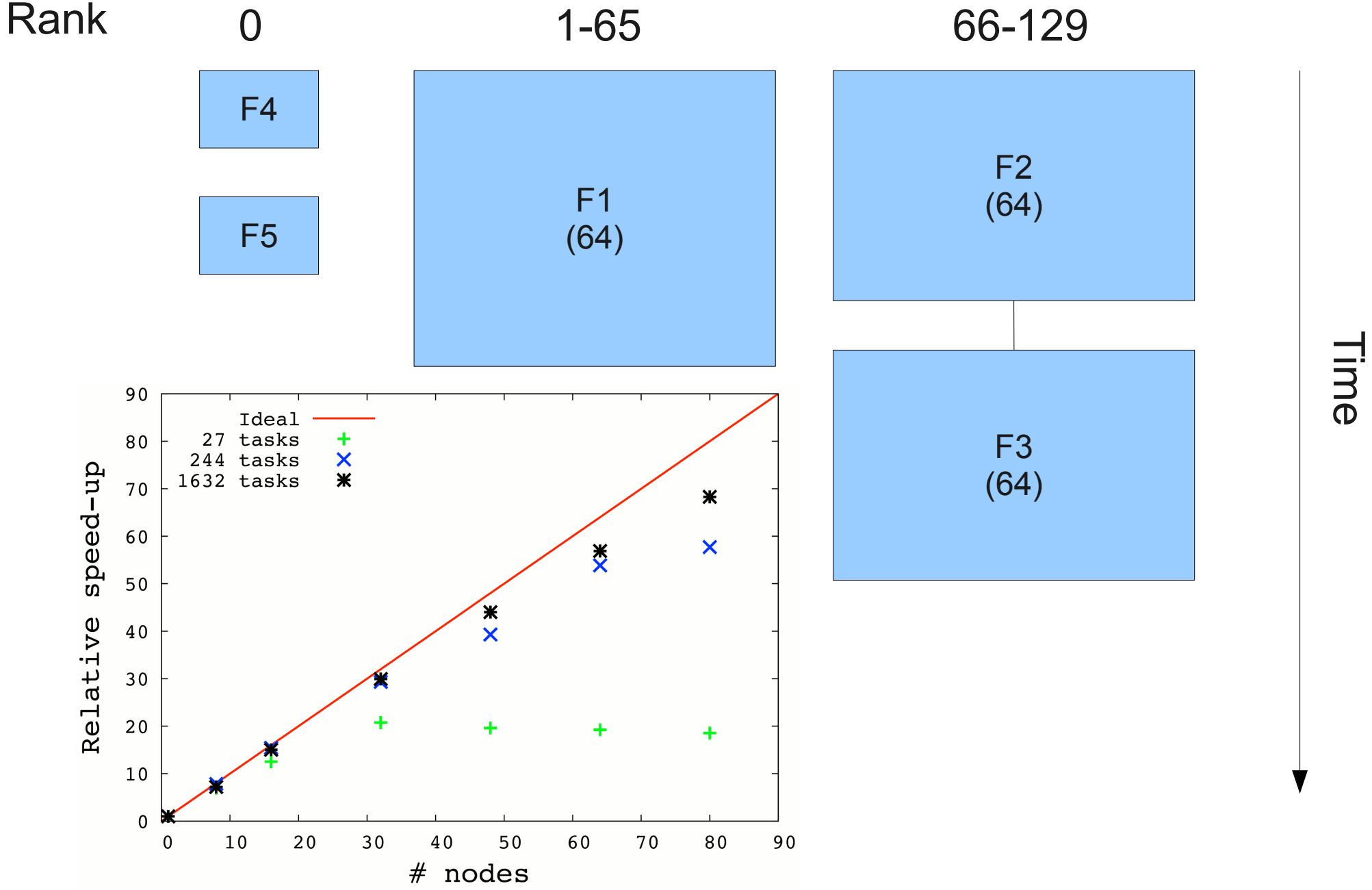
Pair fragment MPI parallelization



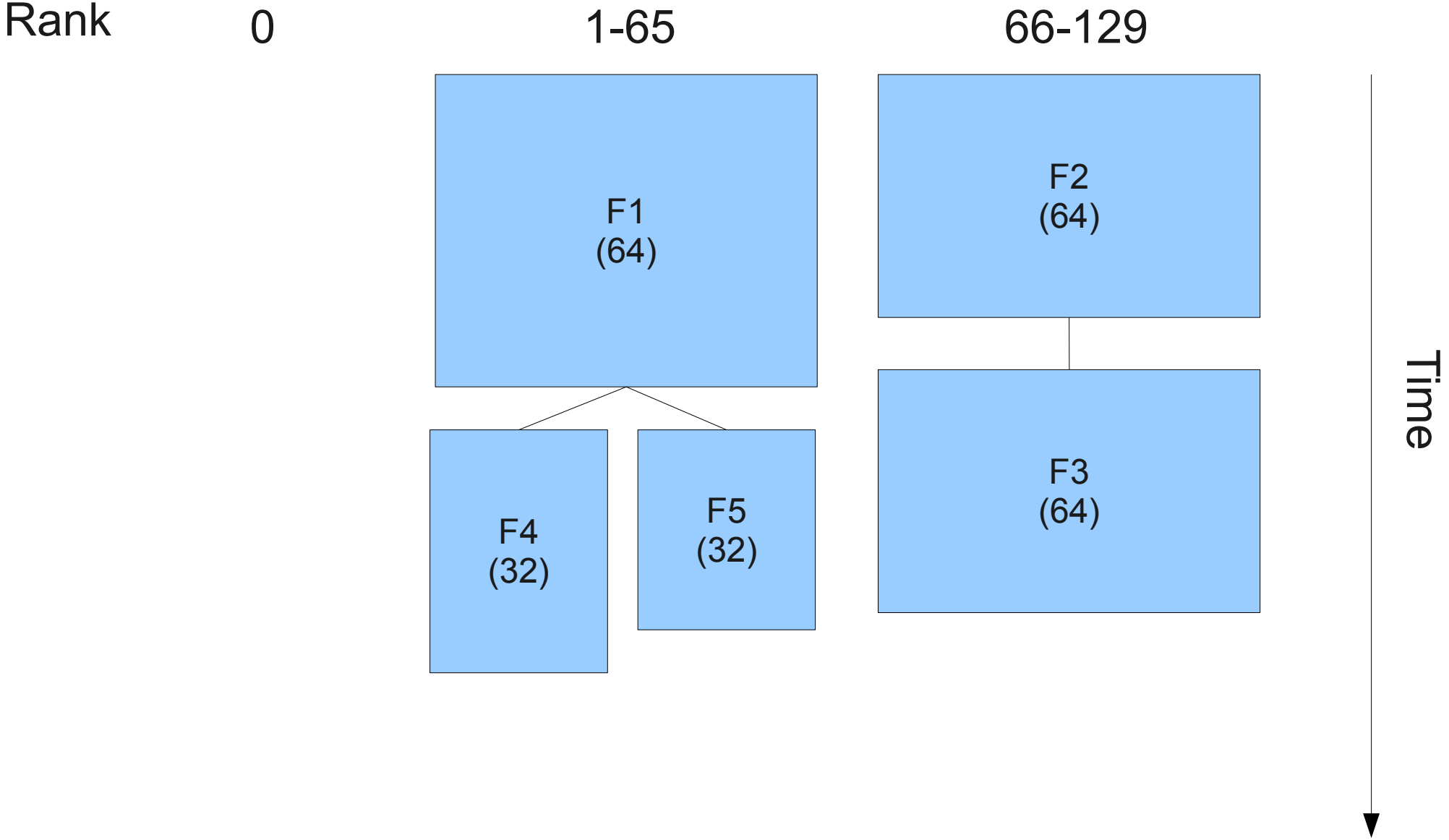
Pair fragment MPI parallelization



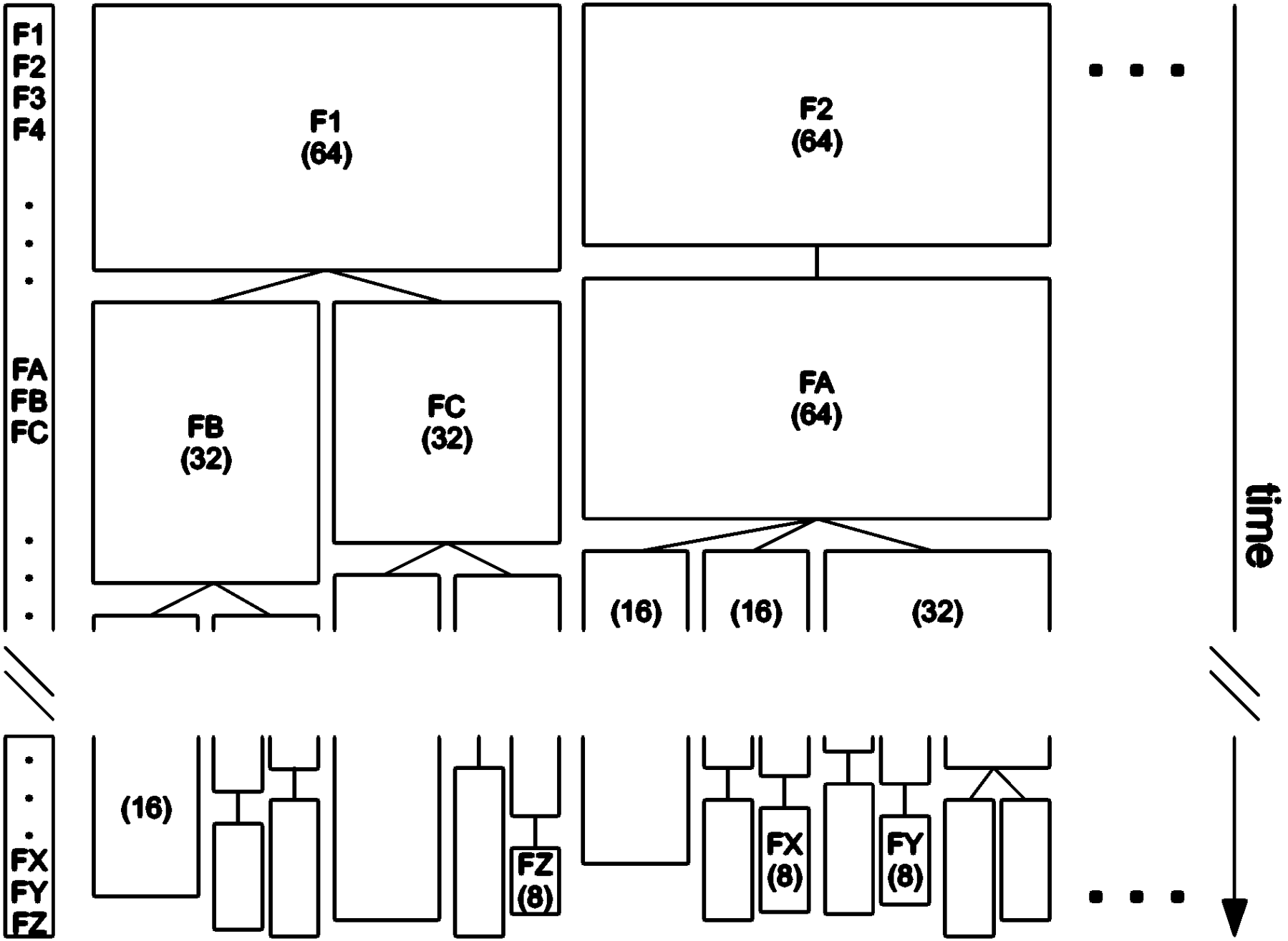
Pair fragment MPI parallelization



Pair fragment MPI parallelization



Pair fragment MPI parallelization

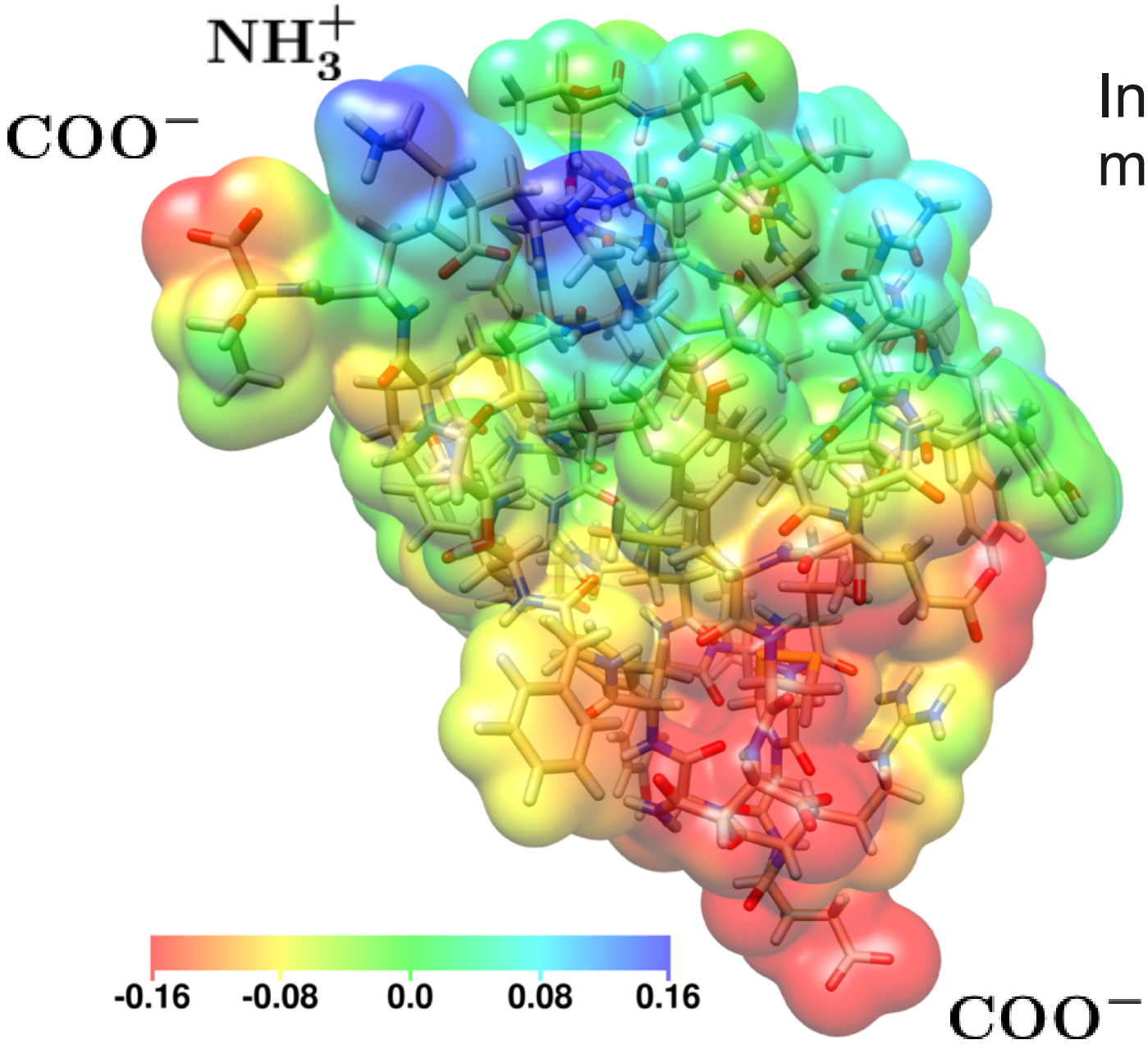


Pair fragment MPI parallelization
Numerical simulation

- 22484 fragments
- Fragment timing from serial calculation (39000 node hours)
- Fragment parallel speedup from sample benchmark
- 282 slots, size 64 (18048 nodes)

- Running time 2.17 wall clock hours
- Average idle time at end: 90 seconds
- 2500+ slots, size 1-16
- **Very good scalability is expected**

MP2 electrostatic potential



Insulin monomer

Goals and Conclusions

- **Perform massively parallel (18000 nodes) MP2/cc-pVDZ calculation on insuline**

- **Show strong scalabiliy and short time to solution**

- Reduced / removed memory bottleneck
- Good parallel speedup for fragment calcuations
- Dynamic load balancing

Discussion toppics

- Skinny matrix multiplication
- Distributed matrix operations on GPU
- Tiled parallelization of the Algorithm
- Fair performance measurement
- PAPI for multiple parallel regions (solved!)

Fragment timing distribution