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JÜLICH
FORSCHUNGSZENTRUM

Efficient parallel I/O

Developing a module for the particle-in-cell code PSC

September 27, 2010 | Axel Hübl

Outline

Motivation and issues with the present configuration

- Part 1: The particle-in-cell code `PSC`

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- Part 2: Output in massiv parallel environments

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- Part 6: Conclusion

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Part I: The particle-in-cell code PSC

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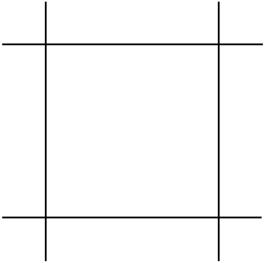
Particle-in-cell codes in general

A short introduction



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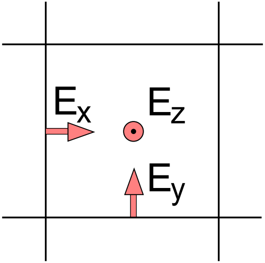

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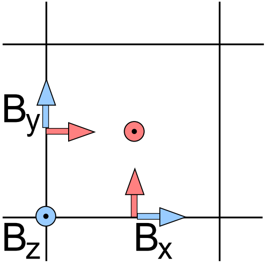

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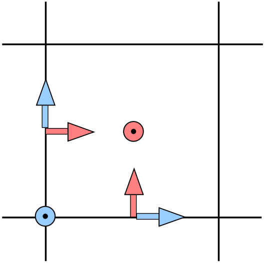

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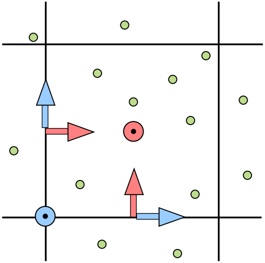

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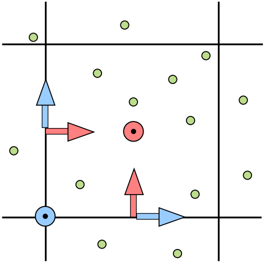
- Particles are smeared on the mesh grids randomly
- Using grid based field and particle solving methods



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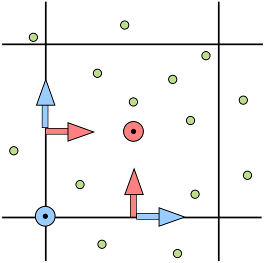

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charges and currents lead to em-fields

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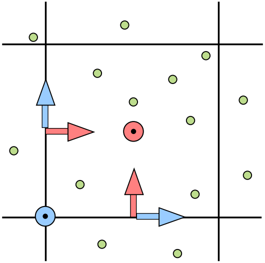

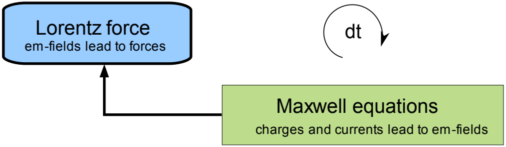

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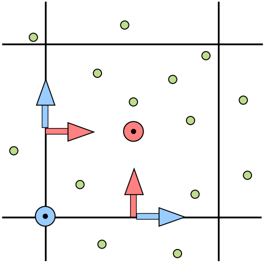

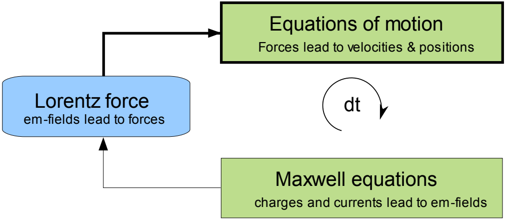

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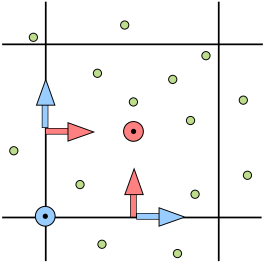

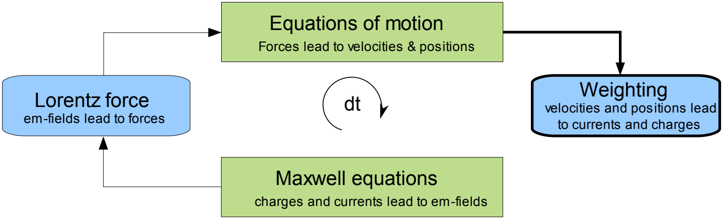

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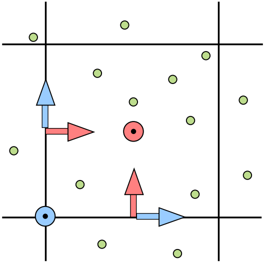

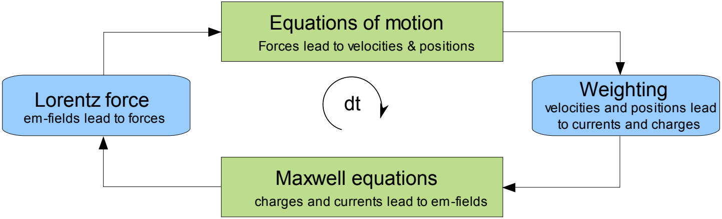

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A mesh-based plasma code

- Major SimLab Plasma physics (SLPP) code for laser-plasma interaction simulations

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- Major SimLab Plasma physics (SLPP) code for laser-plasma interaction simulations
- Originally created by Hartmut Ruhl, LMU, Munich
- Full 3D cartesian mesh based, relativistic em-field solver and particle pusher
- Present optimal usage: up to 1k tasks, with around 15 Million particles (kernel)

The particle-in-cell code `PSC`

Issues with the present I/O

Old I/O

- Puts down the production runs to a great extent

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The particle-in-cell code `PSC`

Issues with the present I/O

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- Puts down the production runs to a great extent
- One file per task and timestep
- Slows down file system
- Files can not be handled any more
- Huge post-processing time

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Efficient parallel I/O

Part II: Output in massiv parallel environments

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Naive implementations

In I/O is ***parallel*.NE.*parallel* !**

- Distributed *global* data set

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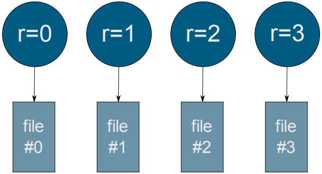

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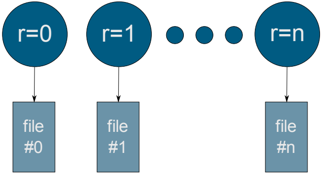

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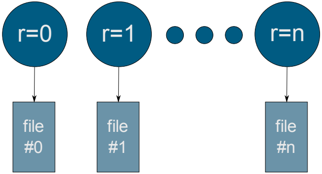

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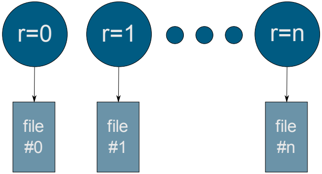

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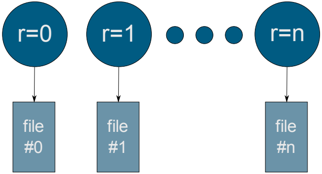

Problems:

- inode limits and post-processing
- file create and delete
- small files and file system block size

Naive implementations

How to handle the output?

- Remove the files of 41 Mio particles

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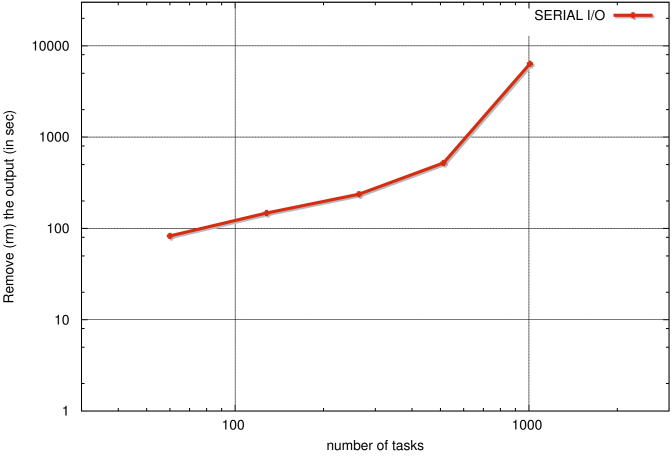

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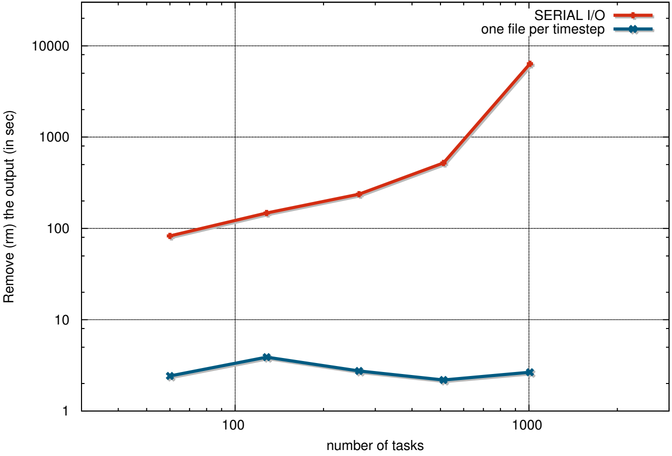

SIONlib

Scalable parallel I/O for task-local files

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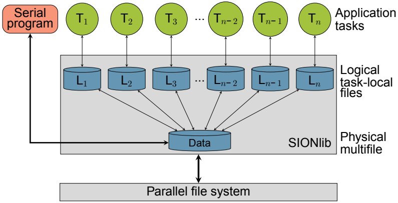

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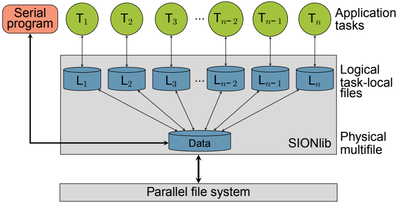

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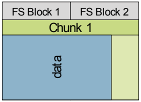

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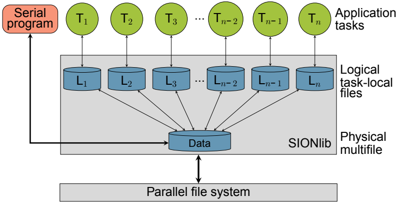

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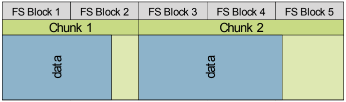

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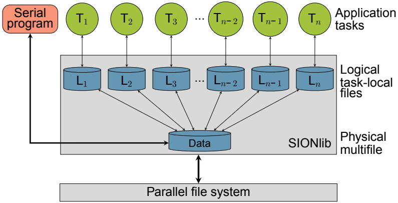

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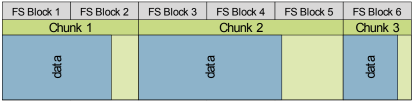

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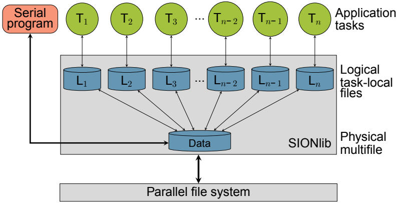

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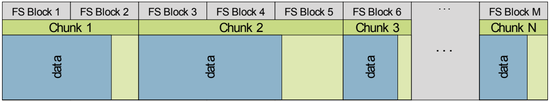

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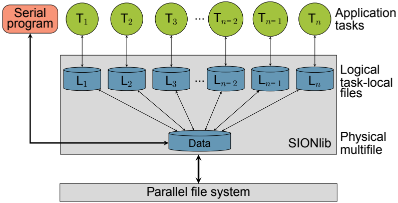

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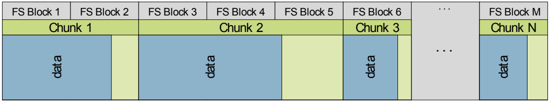

- Support: C, C++, FORTRAN with MPI and OpenMP

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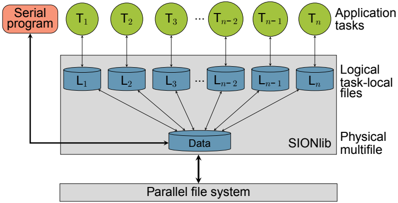

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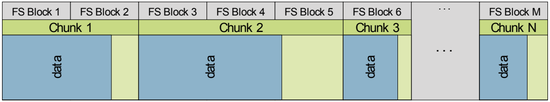

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W. Frings et al.:
Scalable Massively Parallel
I/O to Task-Local Files

www.fz-juelich.de/jsc/sionlib/

MPI-I/O

MPI File extension

- API 1997, part of the MPI standard since 2.0

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MPI File extension

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- Very similar to the message-passing part of MPI
- Presently not useable with LUSTRE file system on Juropa

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Efficient parallel I/O

Part III: New implementation

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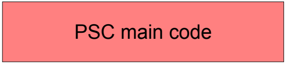
New implementation

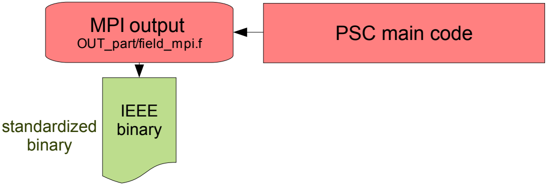
Overview



PSC main code

New implementation

Overview



MPI output
OUT_part/field_mpi.f

PSC main code

IEEE binary

standardized binary

New implementation

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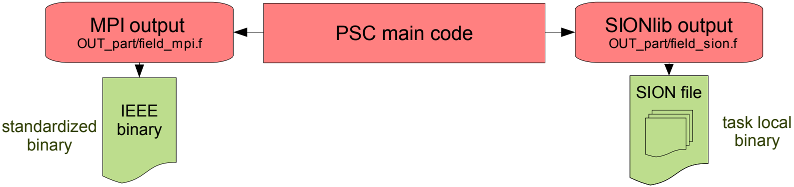

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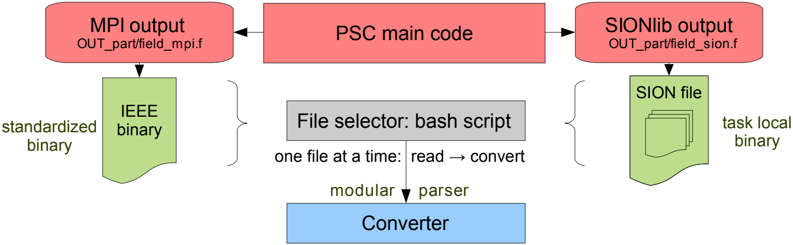

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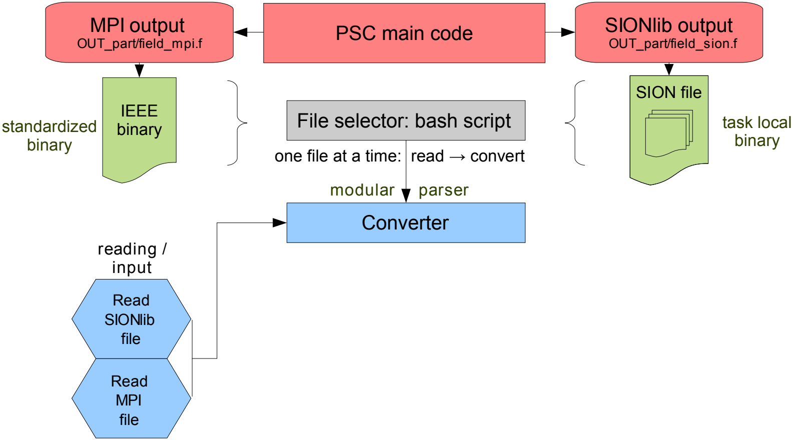

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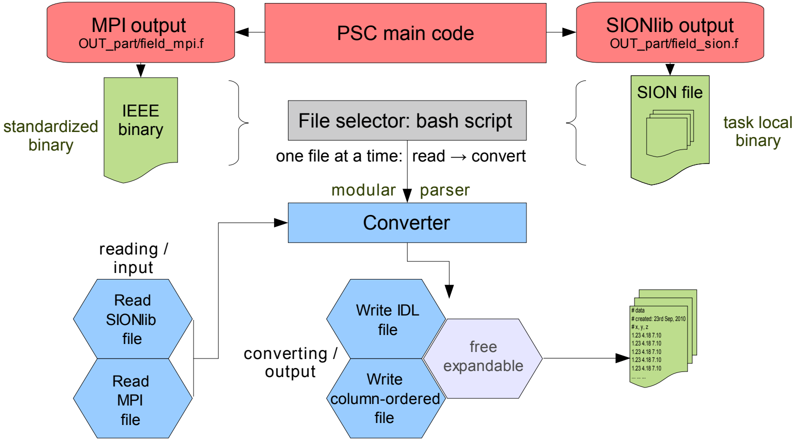


MPI output
OUT_part/field_mpi.f

PSC main code

SIONlib output
OUT_part/field_sion.f

standardized binary

IEEE binary

File selector: bash script

one file at a time: read → convert

SION file

task local binary

modular parser

Converter

reading / input

Read SIONlib file

Read MPI file

converting / output

Write IDL file

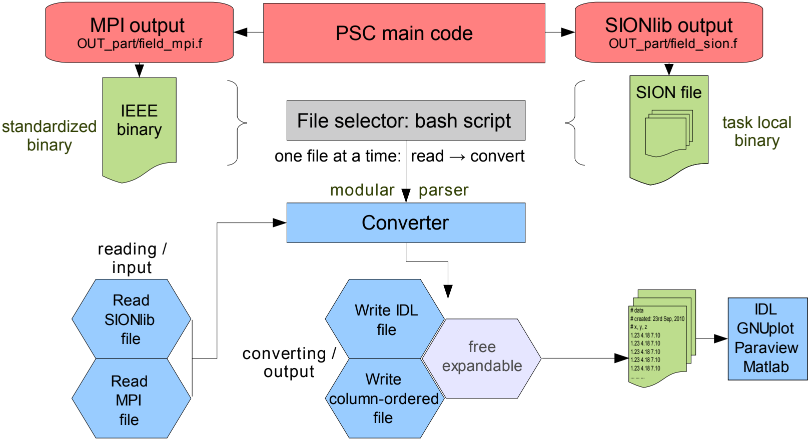
Write column-ordered file

free expandable

```
# data
# created: 23rd Sep, 2010
# x, y, z
1.23 4.18 7.10
1.23 4.18 7.10
1.23 4.18 7.10
1.23 4.18 7.10
1.23 4.18 7.10
... ... ...
```

New implementation

Overview



New implementation

Example of used output commands

SIONlib vs. MPI-I/O

```
call
fsion_paropen_mpi(...)
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```
call MPI_FILE_OPEN(...)
call MPI_FILE_SET_VIEW(...)
```

New implementation

Example of used output commands

SIONlib vs. MPI-I/O

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call fsion_write(
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call MPI_FILE_OPEN(...)
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call MPI_FILE_WRITE_ORDERED(
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call MPI_FILE_CLOSE(...)
```

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Part IV: Post-Processing

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Post-processing

What to do with distributed output?

- Domain decomposition for a field:

Post-processing

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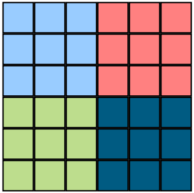
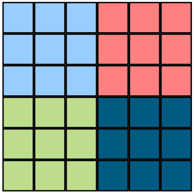
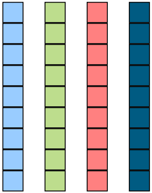


Post-processing

What to do with distributed output?

- Domain decomposition for a field: RAM (Fortran order)





Post-processing

What to do with distributed output?

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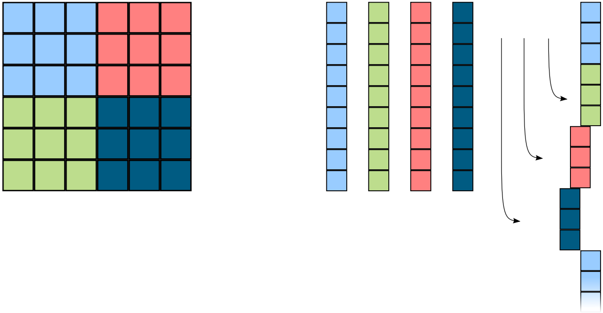

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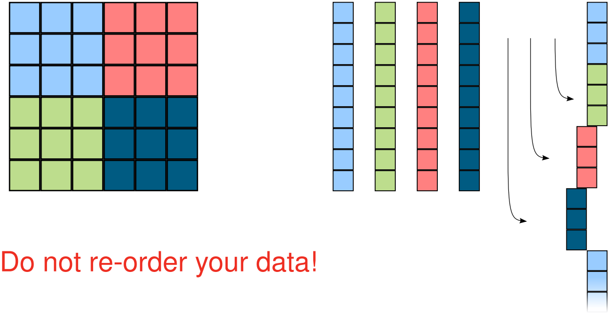

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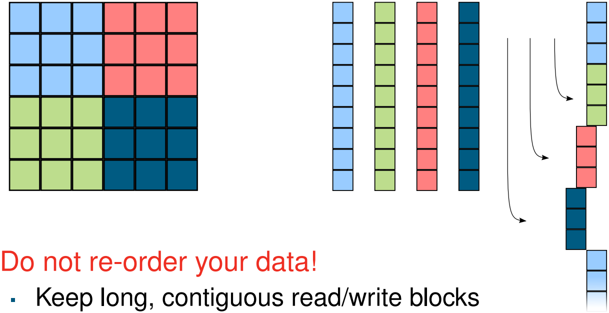

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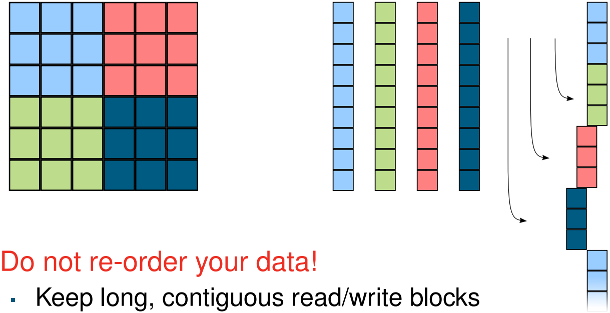

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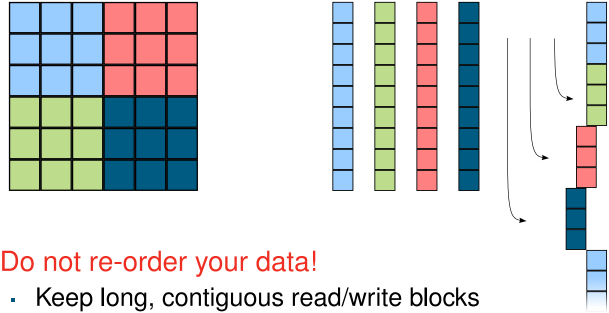

- Do not re-order your data!
  - Keep long, contiguous read/write blocks
  - Result: no temp data, less seeking, no double reading
- Choose a visualization software, that understands decomposition schemes.

Mitglied der Helmholtz-Gemeinschaft

Efficient parallel I/O

Part V: Results

September 27, 2010 | Axel Hübl

Scaling

SIONlib vs MPI-I/O

- Jugene, 19 Mio particles: Data per tasks drastic below 2 MB

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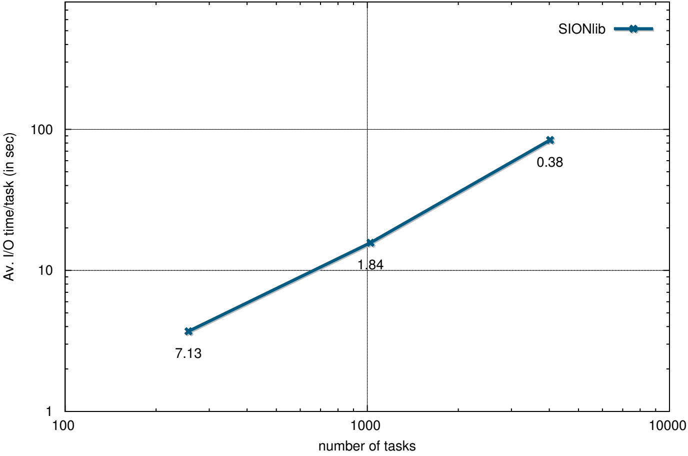

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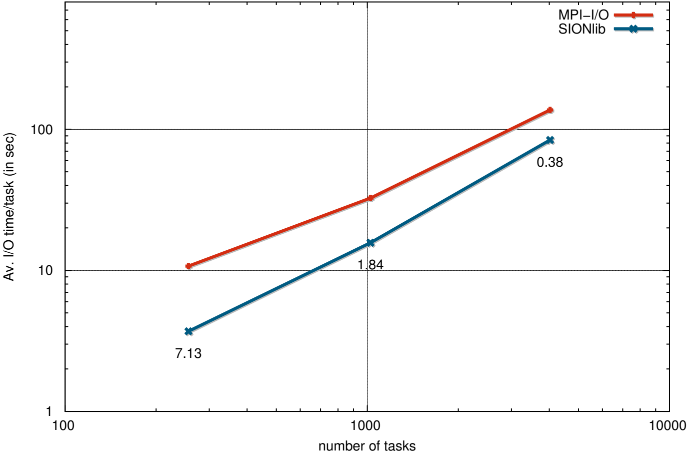

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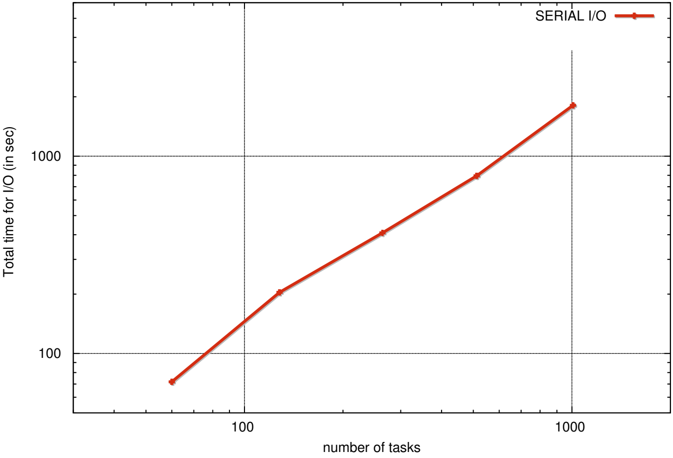

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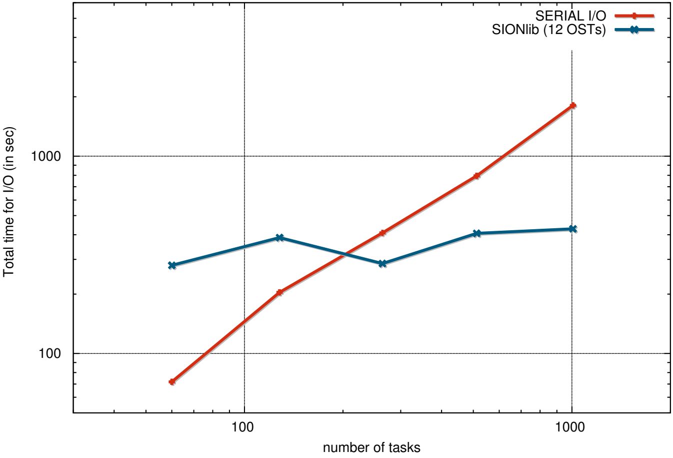

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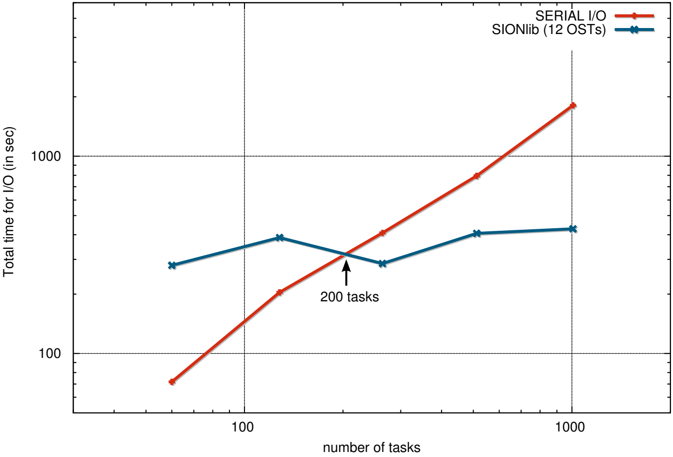

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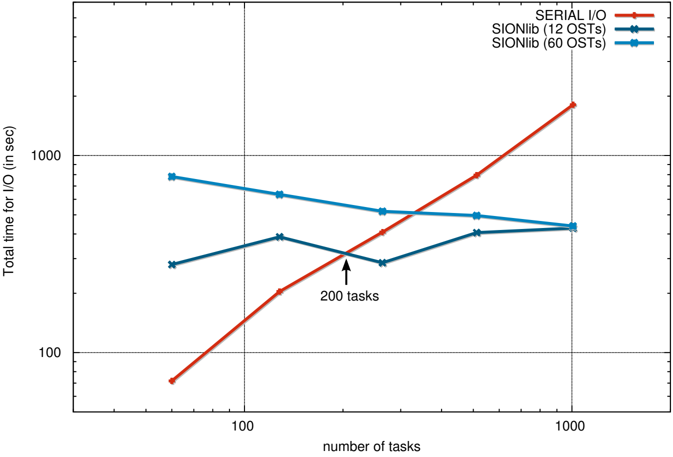

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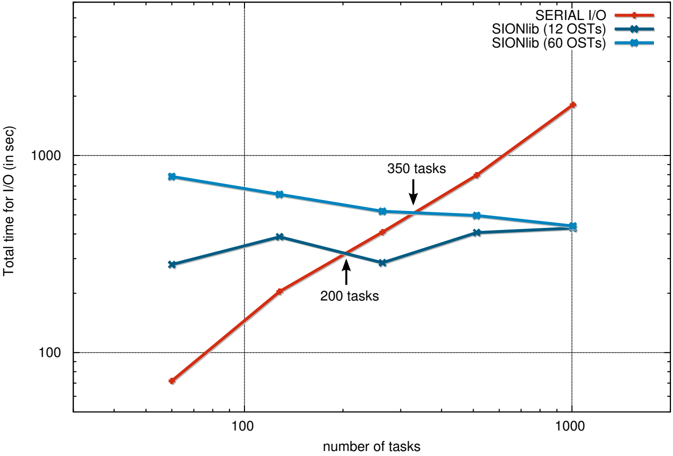

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Post-processing time

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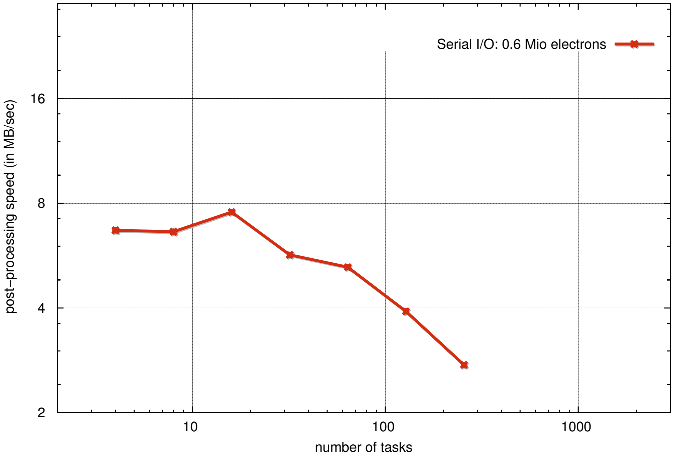

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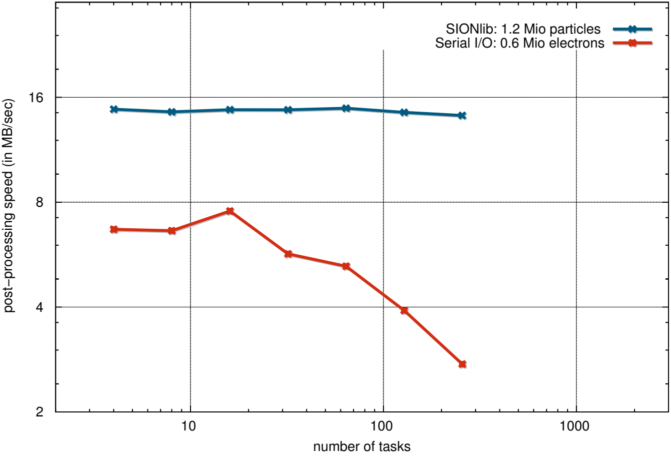

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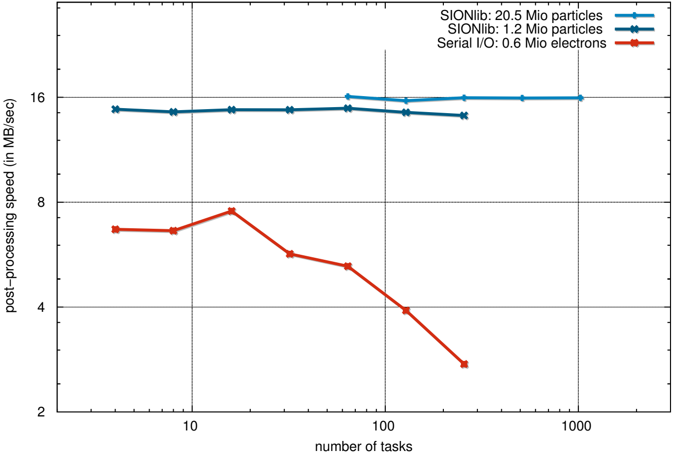

Visualization

Wake field acceleration

- A laser pulse propagates through a plasma

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Efficient parallel I/O

Part VI: Conclusion

September 27, 2010 | Axel Hübl

Conclusion

What is possible now

Achievements

- single file per time step for fields and particles

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- single file per time step for fields and particles
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  - fast post-processing
  - widely supported output formats
- possible parallel visualization through Paraview for large scale/ultra-high resolution productions
- I/O is now ready for future improvements of PSC
- Converters and output modules could also be used for similar projects

Conclusion

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Future prospects

- Checkpointing with SIONlib

Conclusion

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- More converters: hdf5, netcdf, ...

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- visualization scripting for publication quality

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Future prospects

- Checkpointing with SIONlib
- More converters: hdf5, netcdf, ...
- visualization scripting for publication quality
- satisfactory preliminary comparison for the physical output, but microscopical comparison for a set of physical problems needed

Thank you for your attention!

Contact

Author, Disclaimer

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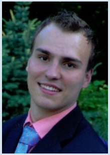
- Physics student (Diploma)
- axel.huebl _at_ web.de



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