A new concept for efficiently parallelizing PIC codes in plasma physics

R. Hatzky

1. Introduction
2. Structure of a PIC code
3. Optimization on RISC processors
4. Particle counting sort
5. Performance on an IBM 'Regatta' node
6. Decomposition techniques
7. Parallelization of the field solver
8. Summary

Introduction I

Particle-in-cell (PIC) codes are widely used for modeling many body systems, as e.g. in

- **plasma simulations**
- **semiconductor device simulations**
- **gravitational N-body problems**

The number of physical particles N_S in a plasma physics simulation is usually too large to be simulated directly.

A PIC code simulates the motion of N macro particles representing each many physical particles ($N \ll N_S$).

Especially nonlinear simulations are computationally very expensive with $N \approx 10^8$ macro particles and a restrictive time step.

Introduction II

Example: the plasma physics PIC codes TORB[1]/ORB5[2] to simulate the time evolution of ion-temperature-gradient-driven (ITG) turbulence in cylindrical/tokamak geometry:

- **The numerical method is a particle-mesh method.**
- **The macro particles sample the five-dimensional reduced phase space.**
- **A mesh is needed to calculate the three-dimensional spatial electrostatic potential.**

Minimum number of macro particles: $134 \cdot 10^6$

The smallest mesh size (r, θ, z)**:** $67 \times 259 \times 35$

[1] **R. Hatzky, et al.,** *Phys. Plas.*, **9, 898 (2002).**
[2] **S. Jolliet, et al.,** *Comp. Phys. Commun.*, **in press (2007)**

Structure of a PIC Code

For each time step the electrostatic PIC code executes three main parts:[1]

- **Charge deposit (accumulation)** $\approx 40\ \%$
- **Field solve** $< 5\ \%$
- **Electric field calculation** $\approx 45\ \%$
  + time integration (push) $\approx 5\ \%$

The field solve is done by a direct solver with a Cholesky decomposition done at the initialization.

The macro particle communication for a typical 32 **processor run takes** $\approx 5\ \%$**.**

A typical counting sort of the particles takes $\approx 5\ \%$**.**

[1] **V. K. Decyk,** *Comp. Phys. Comm.*, **87, 87 (1995).**

Optimization on RISC Processors

General optimization strategies:[1]

- **Storing particle components together in one array.**
- **Sorting particle and field components together.**
- **Removing `IF` statements by using guard cells.**

Cache based RISC architecture:

Cache trashing occurs when the charge and/or electric field array do not fit into the cache.

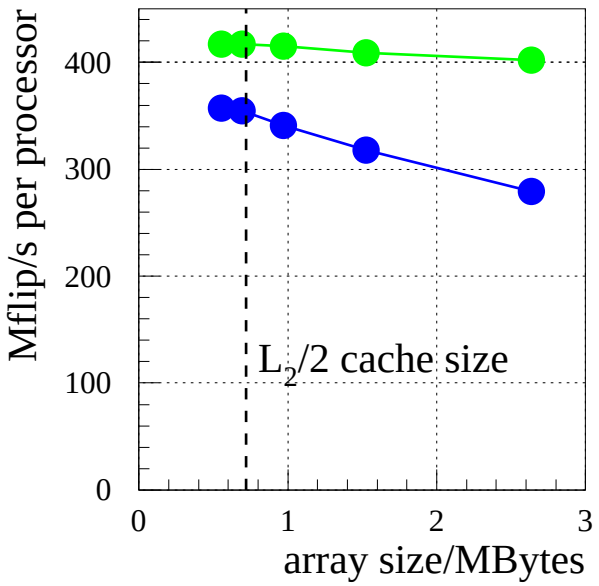
A maximum cache reuse is given when all the particles in the same mesh cell are processed together.

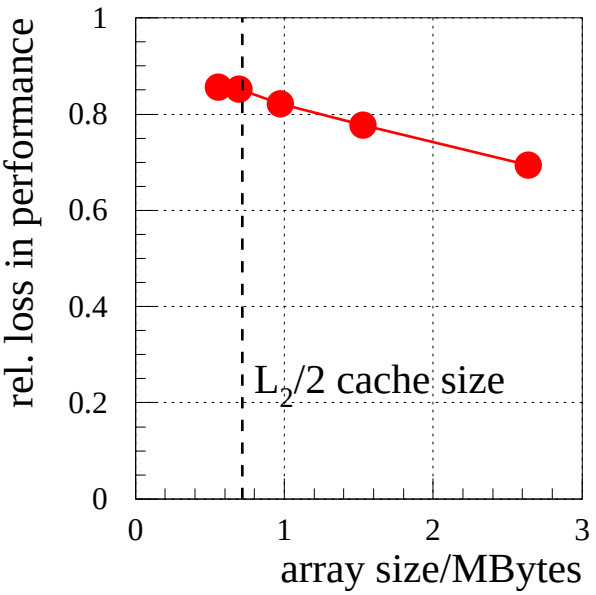
Solution:

Counting sort of the particles into the bins of the grid.

[1] **V. K. Decyk, et al.,** *Comp. Phys.*, **10, 290 (1996).**

Particle counting sort

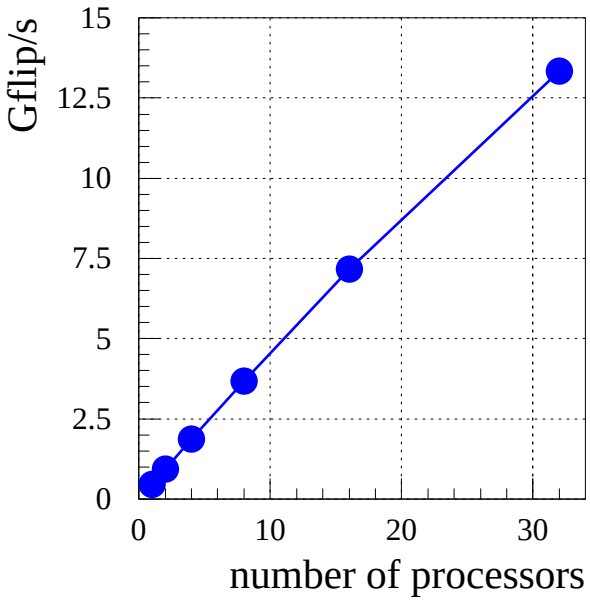


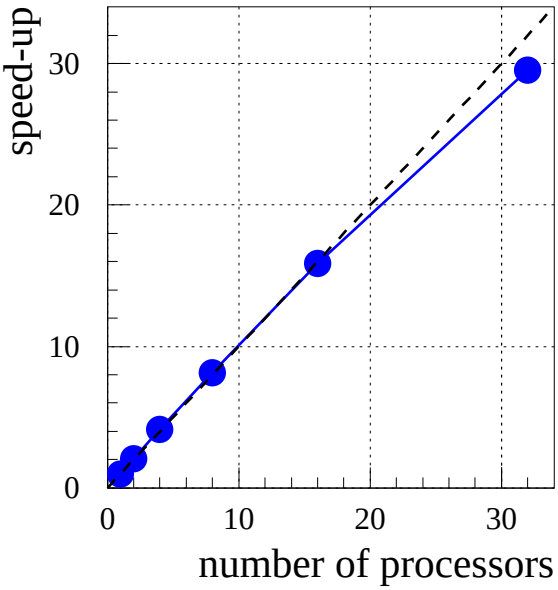


Degradation of the performance with larger array size due to the cache architecture of the IBM Power4 processor:

- **Degradation starts at** $\approx L_2/2 = 0.72$ **MBytes**
- **Only slight degradation with particle sort**
- **Rel. performance loss without particle sort** $> 30\ \%$
- **Already gain of** $\approx 15\ \%$ **for small arrays**

Performance on an IBM 'Regatta' node





Communication of the particles among the processors (IBM Power4) only in large packages:

- **Nearly perfect scaling for ≤ 16 processors**
- **Overall speed-up of ≈ 29**

$\Rightarrow$ good scalability with the number of processors.

But only $\approx 12\ \%$ of the peak performance.

Decomposition techniques I

Domain decomposition:

Different portions of the physical domain are assigned to different processors, including the particles and field data that reside on them.

Advantage:

- **The field data are local**
  $\Rightarrow$ small memory consumption.

Disadvantages:

- **The particles have to be communicated among the subdomains (processors).**
- **The number of neighboring subdomains scales with the number of processors:**
  $\Rightarrow$ the spatial extent in the direction of parallelization becomes smaller and smaller.
  $\Rightarrow$ the particle communication is increased; the minimal grid resolution is increased.

Decomposition techniques II

Particle decomposition:

The whole spatial grid is assigned to each processor, which takes care only of a subset of the particles.

Advantages:

- **Intrinsic load balancing**
- **No particle communication**
- **Moderate effort in porting existing sequential programs into parallel form**

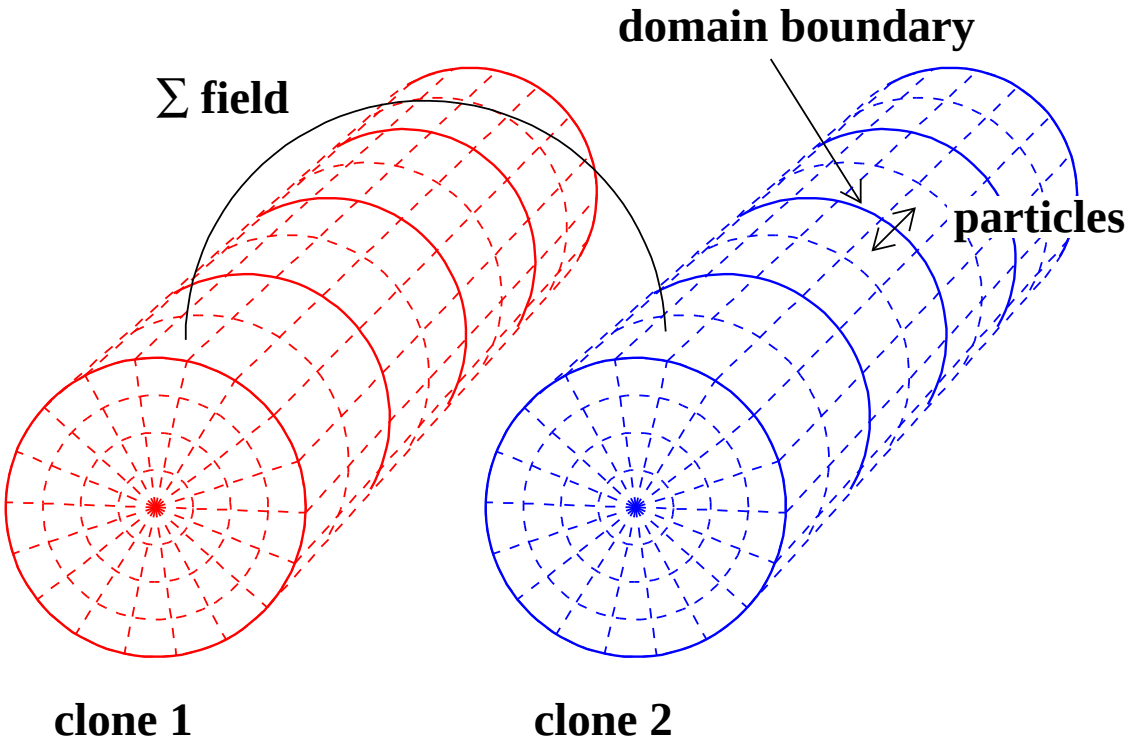
Disadvantages:

- **A global reduction communication for the field data.**
- **The field data have to be stored on each processor $\Rightarrow$ high memory consumption.**
- **A large average number of particles per grid cell on the single processor is needed (cache reuse).**

Decomposition techniques III

Domain cloning:[1]

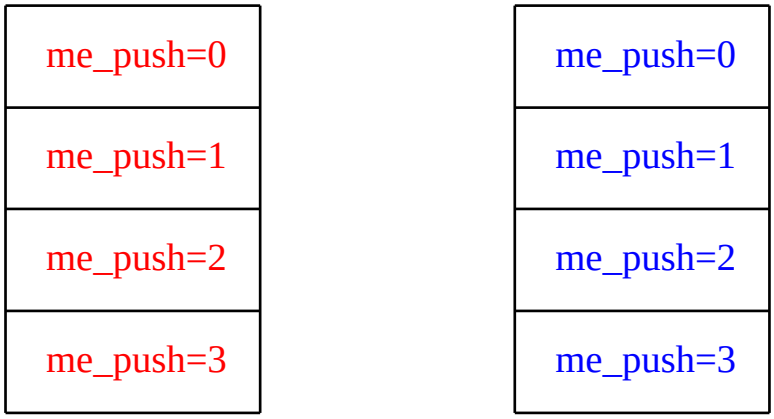
The simulation domain is cloned, i.e. multiple copies of the same domain are made.



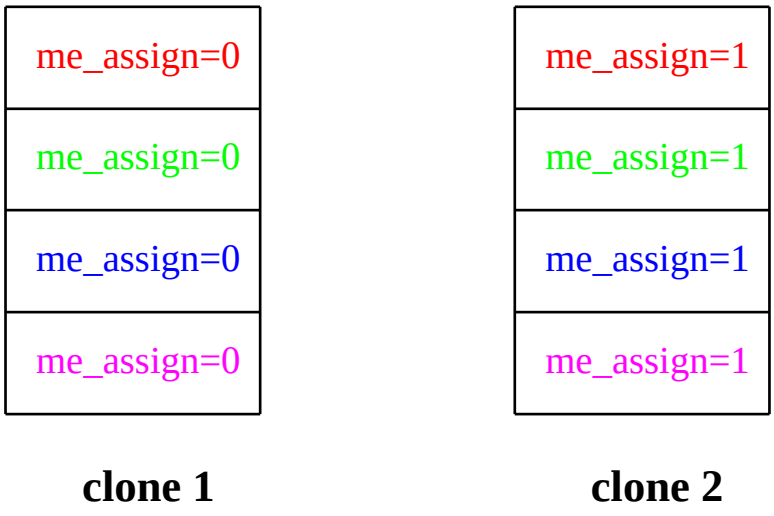
[1] **C. C. Kim and S. E. Parker,** *J. Comp. Phys.*, **161, 589 (2000).**

Decomposition techniques IV

Particle MPI communicator comm_push



Charge-assignment MPI communicator comm_assign



Decomposition techniques V

General advantages:

- **Domain decomposition and particle decomposition are included as limiting cases.**
- **No correlation between grid resolution and number of processors.**
- **The implementation can be easily performed as a supplement to one-dimensional domain decomposition.**

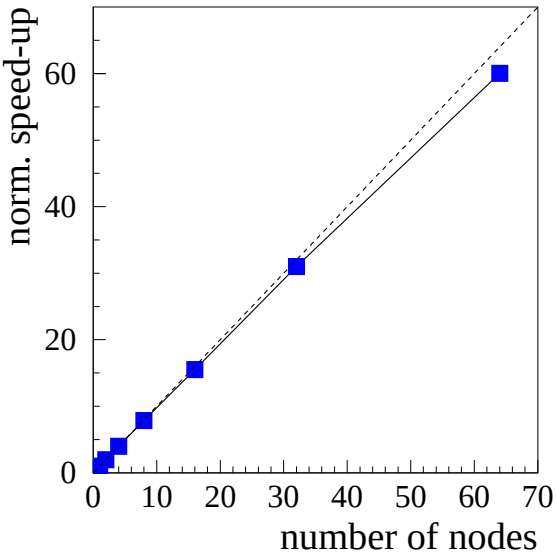
Possible advantages on a clustered SMP computer:[1]

- **Dominating particle communication inside a node $\Rightarrow$ occurs on the fast shared memory.**
- **Moderate field communication between the nodes $\Rightarrow$ passes the slower network (IBM Federation switch).**

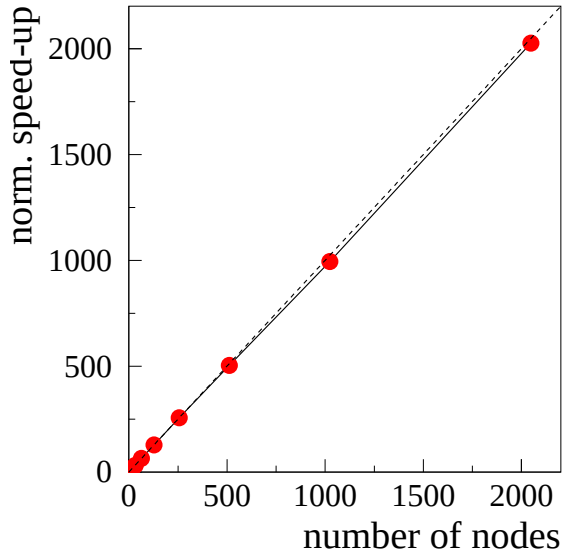
[1] **R. Hatzky,** *Parallel Computing*, **32, 325, 2006.**

Decomposition techniques VI

ECMWF TORB run on IBM pSeries 690+ servers (node) each of which has 32 1.9 GHz Power 4+ CPUs:



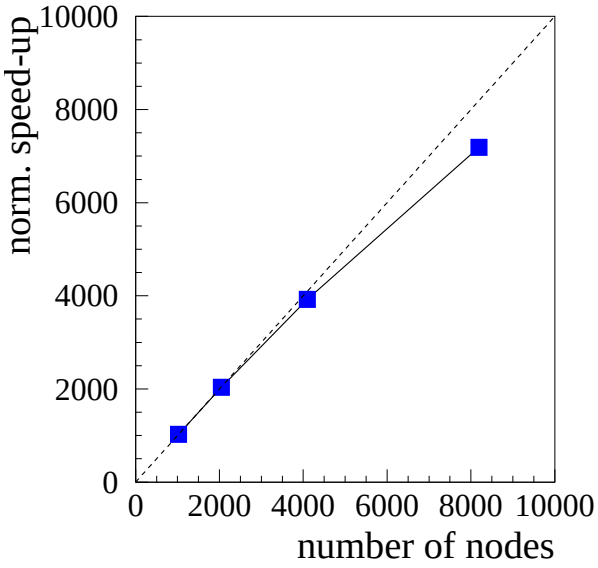
BSC TORB run on 2.2 GHz IBM Power PC 970FX dual blade nodes:



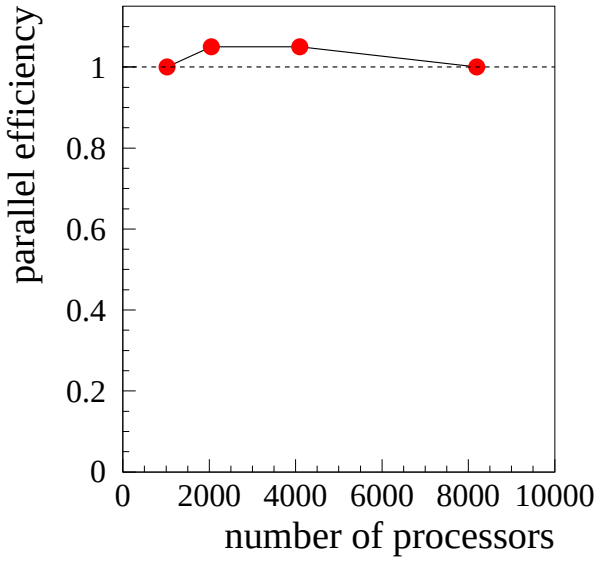
Decomposition techniques VII

IBM Watson Research Center `ORB5` runs on IBM Blue Gene/L with 0.7 GHz PowerPC 440d CPUs

strong scaling:



weak scaling:



Field solver I

3D matrix is transformed by an FFT decomposition in toroidal direction into a system of 2D matrix equations.

Advantage:

- **Trivial parallelization on each clone over the Fourier modes.**

Disadvantage:

- **2 FFT's per field solving** $[\mathcal{O}(N \log_2 N)]$

Using the MPI communicator comm_assign for parallelization of the field solving.

Advantage:

- **Parallelization over the clones avoids redundant field solving.**

Disadvantage:

- **The factorized and parallelized matrix has to be stored several times $\Rightarrow$ conflicts memory limitation.**

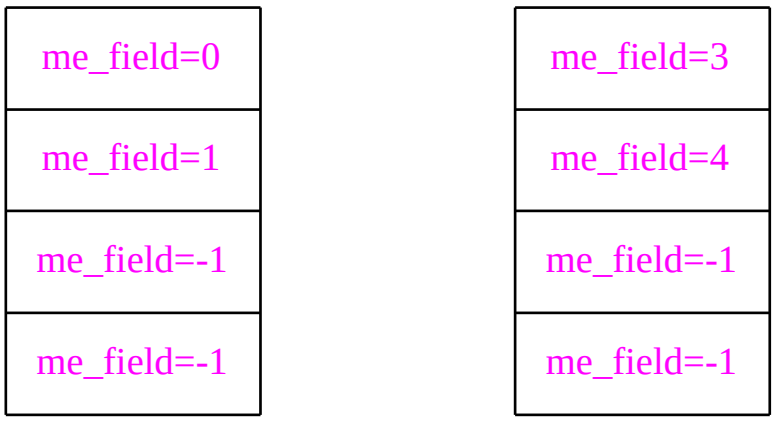
Field solver II

Especially for large matrices a third MPI communicator comm_field has to be defined which is completely independent from the domain cloning concept.

Advantage:

- **Maximal flexibility to adapt to the scaling properties and memory consumption of the chosen parallel solver.**

Field solver MPI communicator comm_field



Field solver III

The ORB5 code solves simultaneously:

1. **a sparse Helmholtz equation for ϕ using the MPI communicator comm_assign**
2. **a dense integro-differential equation for $\bar{\phi}$ using the MPI communicator comm_field**

Benchmarks with two direct solvers have been done for a 3D grid with:

1. **the publicly available library ScaLAPACK for dense matrices**
2. **the commercial IBM library WSMP for sparse matrices**

on an IBM 'Regatta' node with 32 processors and 4 clones.

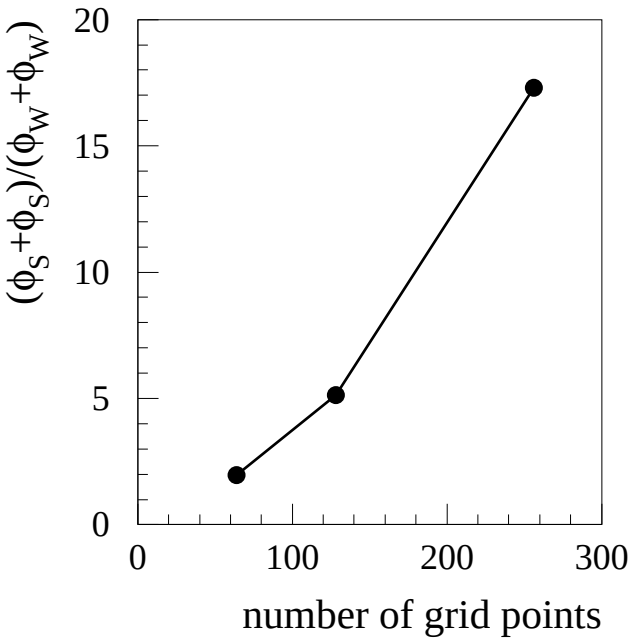
Watson Sparse Matrix Package (WSMP)

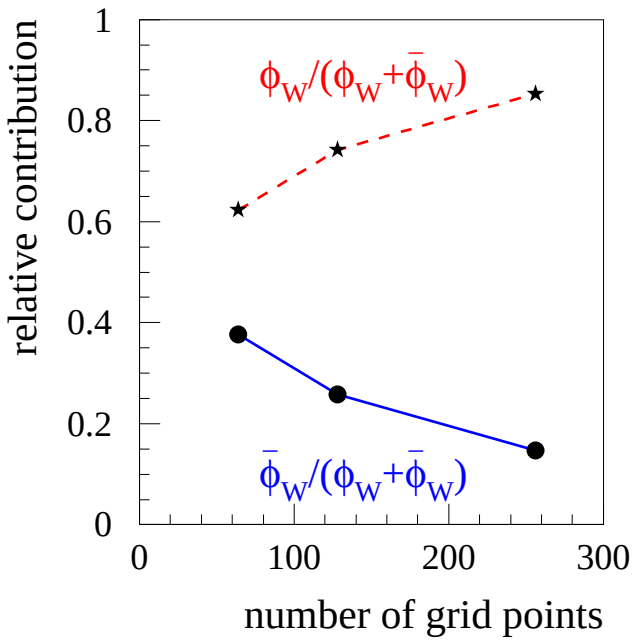
The IBM Watson Sparse Matrix Package, WSMP, is a high-performance software package for solving large sparse systems of linear equations using a direct method:

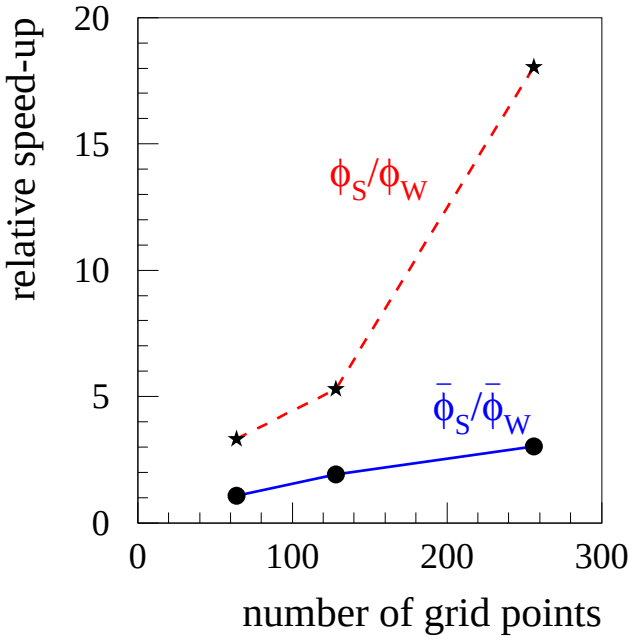
Advantages:

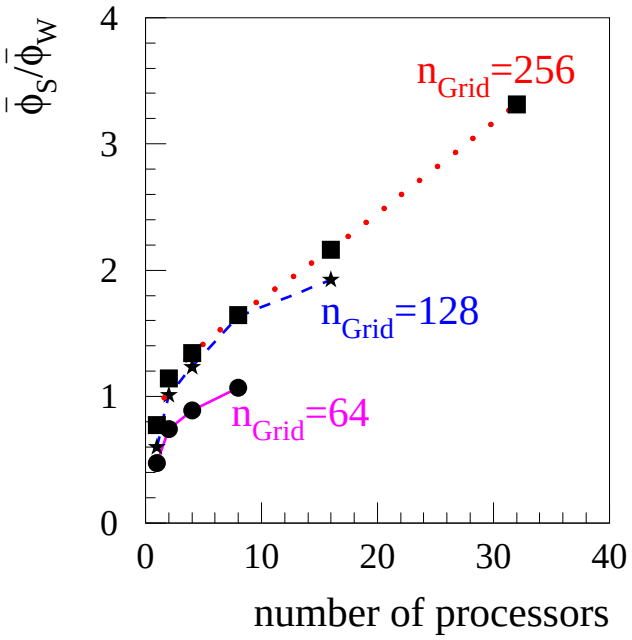
1. **can be used as a serial package, or in a shared-memory multiprocessor (SMP) environment, or as a scalable parallel solver in a message-passing (MPI) environment**
2. **shows very good scalability**
3. **is available for AIX and Linux platforms**
4. **is continuously improved by its developer Anshul Gupta who does an excellent job**

Benchmark ScaLAPACK vs. IBM WSMP









Summary

- A particle counting sort enhances the performance on the IBM POWER4 microarchitecture due to a better cache reuse.

  Especially for large charge and/or electric field arrays, which do not fit into the L_2 cache, a performance gain of > 30 % is possible.

- The domain cloning decomposition concept decouples the grid resolution from the number of processors used.

  Good scaling property of 88 % up to 8192 (IBM Watson Research Center) for strong scaling and optimal scaling property for weak scaling could be achieved for the `ORB5` code.

- The IBM WSMP library seems to be the optimal choice to solve for large sparse matrices.