Optimizing Geometry Routines for (SIMD) Vector Particle Tracking

-- goals, challenges, and first results --

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Motivation

- Today, many code optimization efforts target **multicore/threading**
  - For example in simulation software: looking forward to **multithreaded Geant4** (Geant4-MT) coming in the next release

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  - For example in simulation software: looking forward to **multithreaded Geant4** (Geant4-MT) coming in the next release
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- In simulation, some efforts start(ed) thinking **beyond threading**:
  - e.g., "Geant Vector Prototype" (F. Carminati et al.)
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- In simulation, some efforts start(ed) thinking **beyond threading**:
  - e.g., "Geant Vector Prototype" (F. Carminati et al.)
  - GPU simulation prototype (P. Canal et al., Fermilab)
- basic idea: from processing of **single particles** to **vectors of particles**

⇒ **data parallelism**

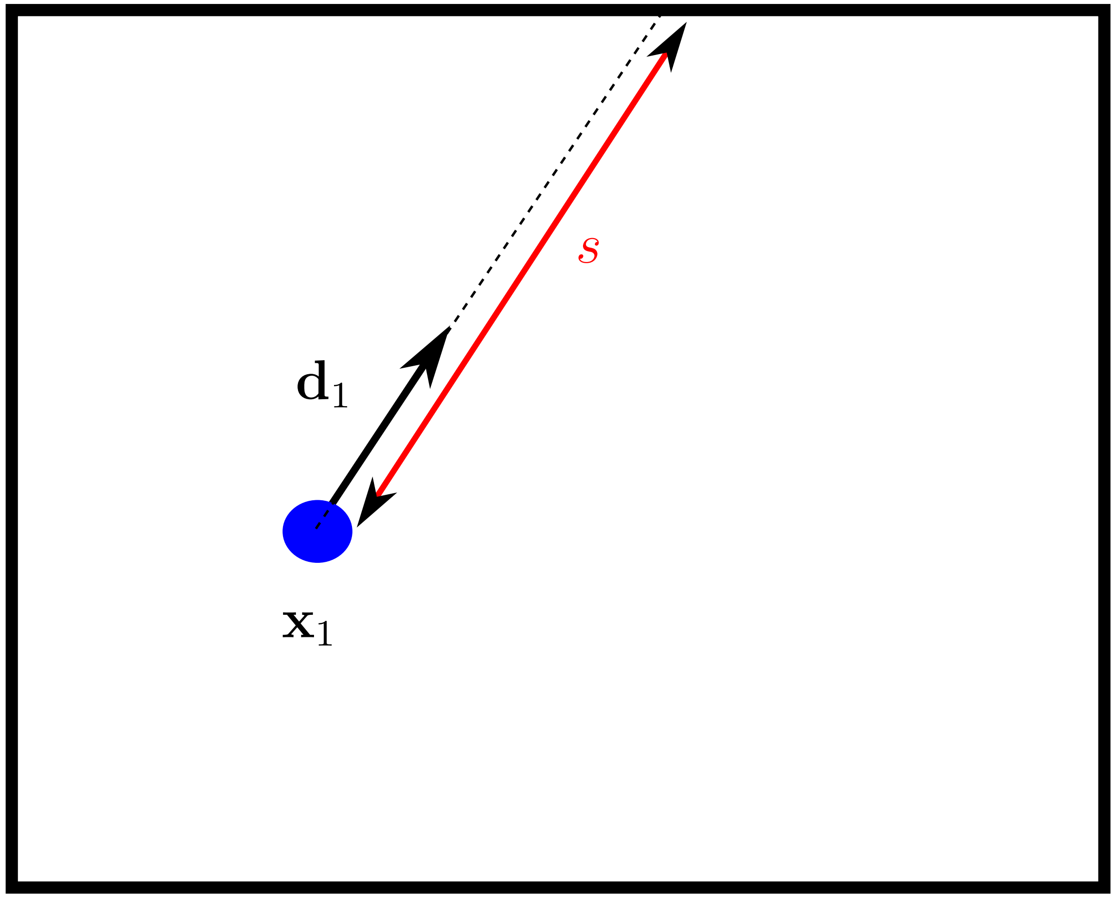
⇒ * **use of SIMD instructions, GPU**

⇒ * **benefit from less cache misses**

TGeoBBox: Example of Vector Processing

- typical geometry task in particle tracking: **get distance to boundary**

```
double
Box::DistFromInside(double *x, double *d);
```



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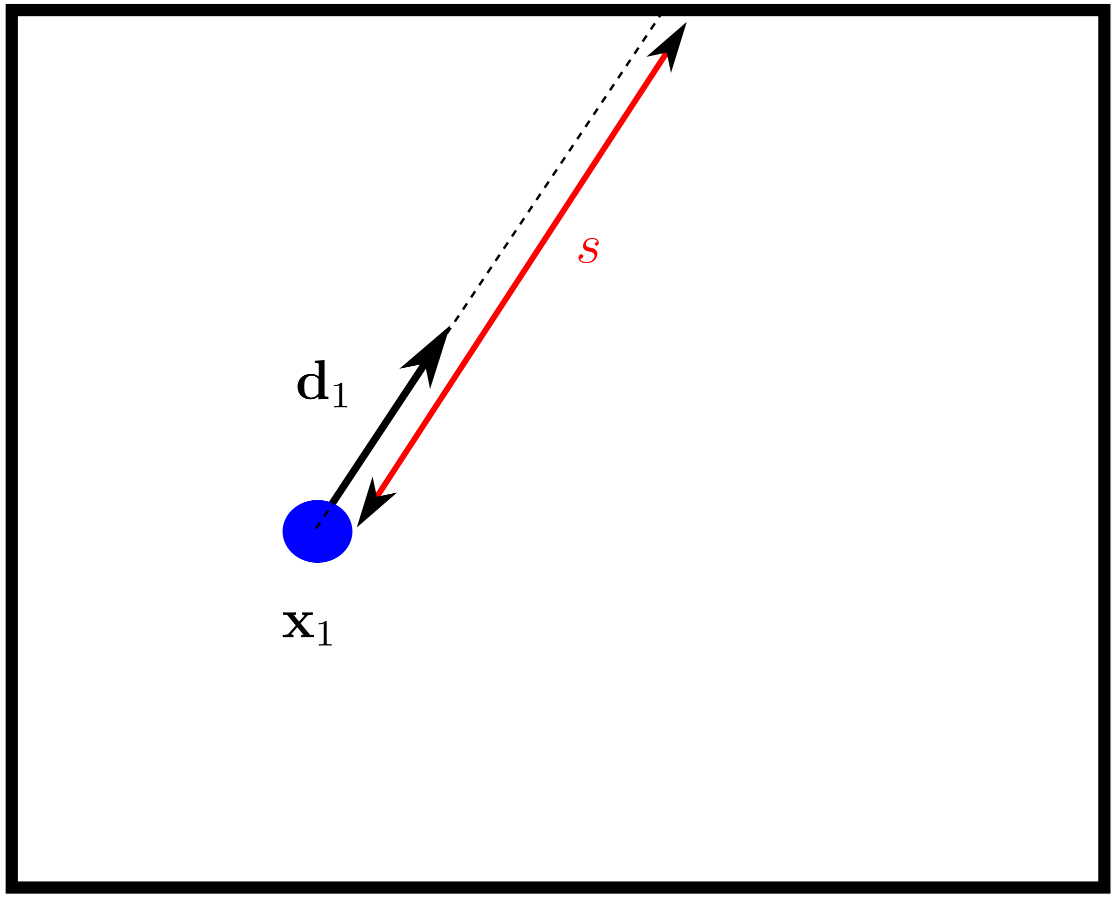
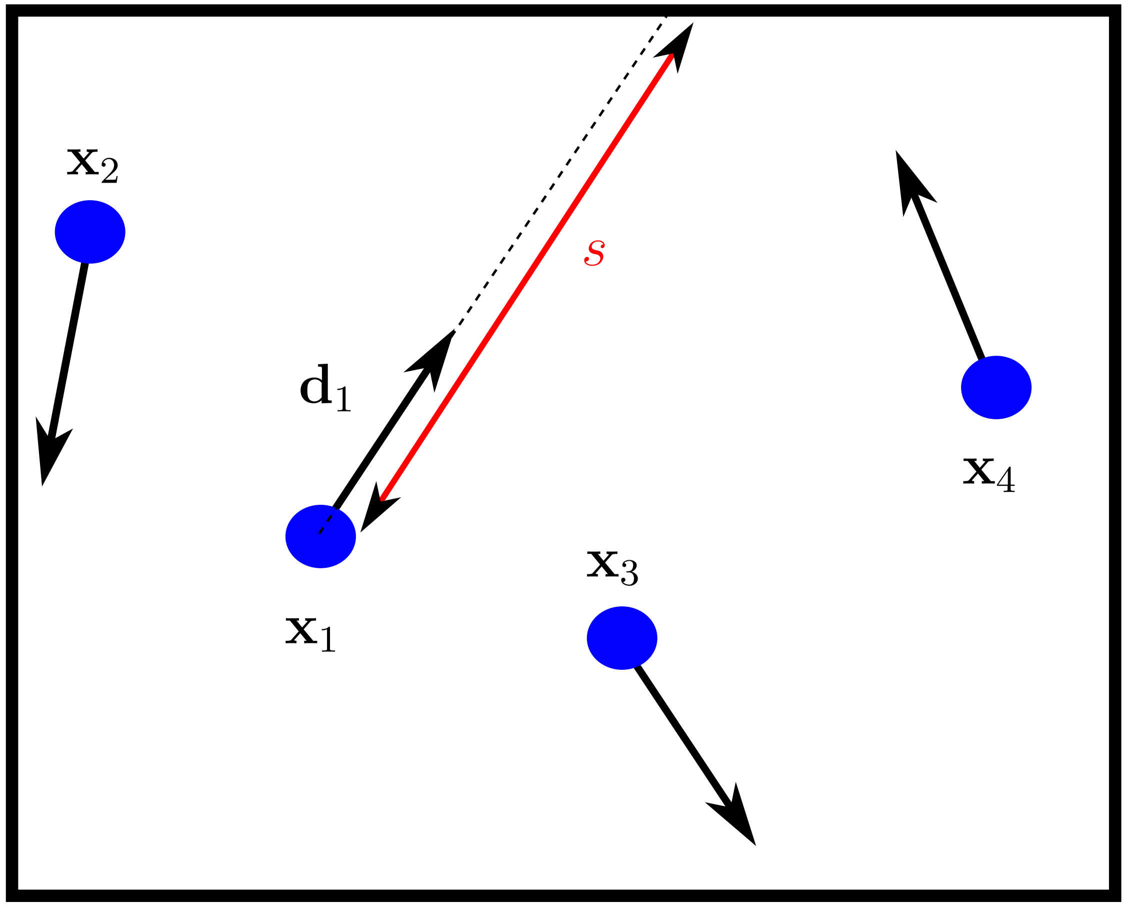


1 particle

```
void
Box::DistFromInside_v(double *x,
double *d, double *dist, int np);
```



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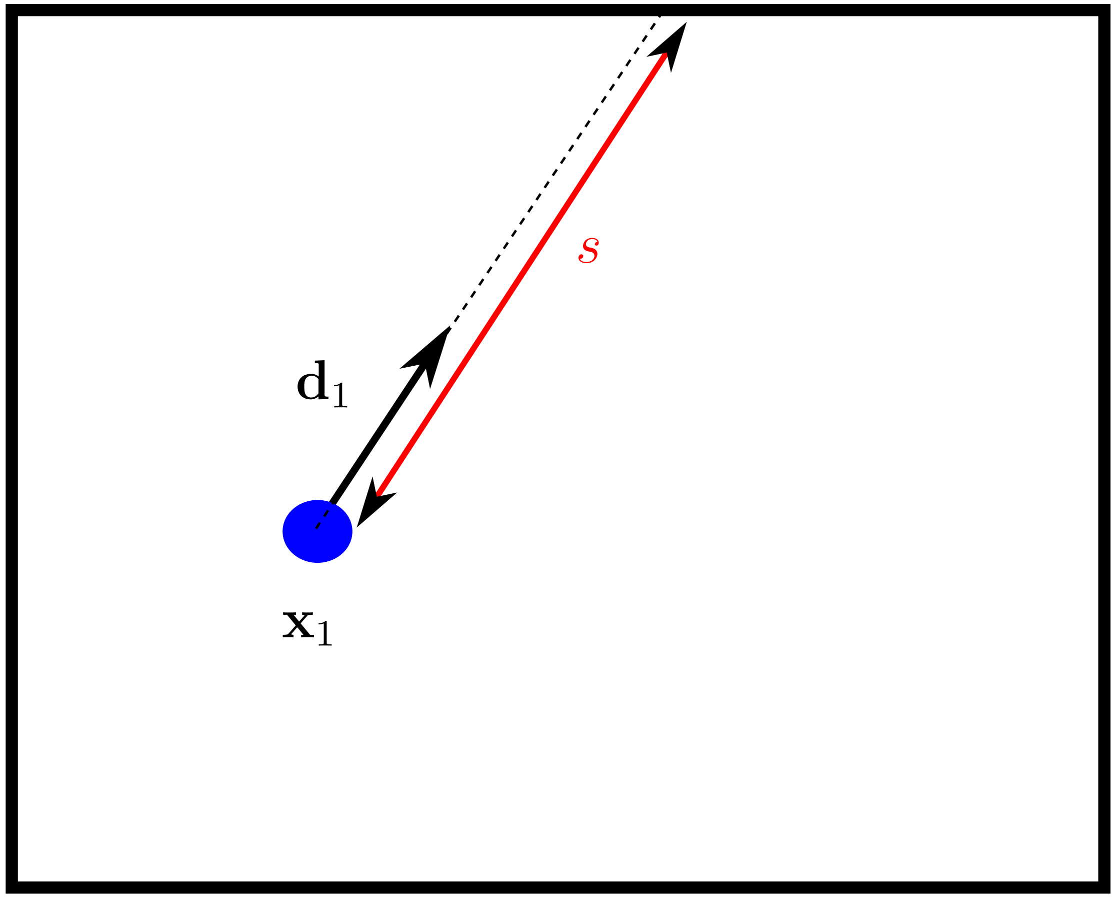

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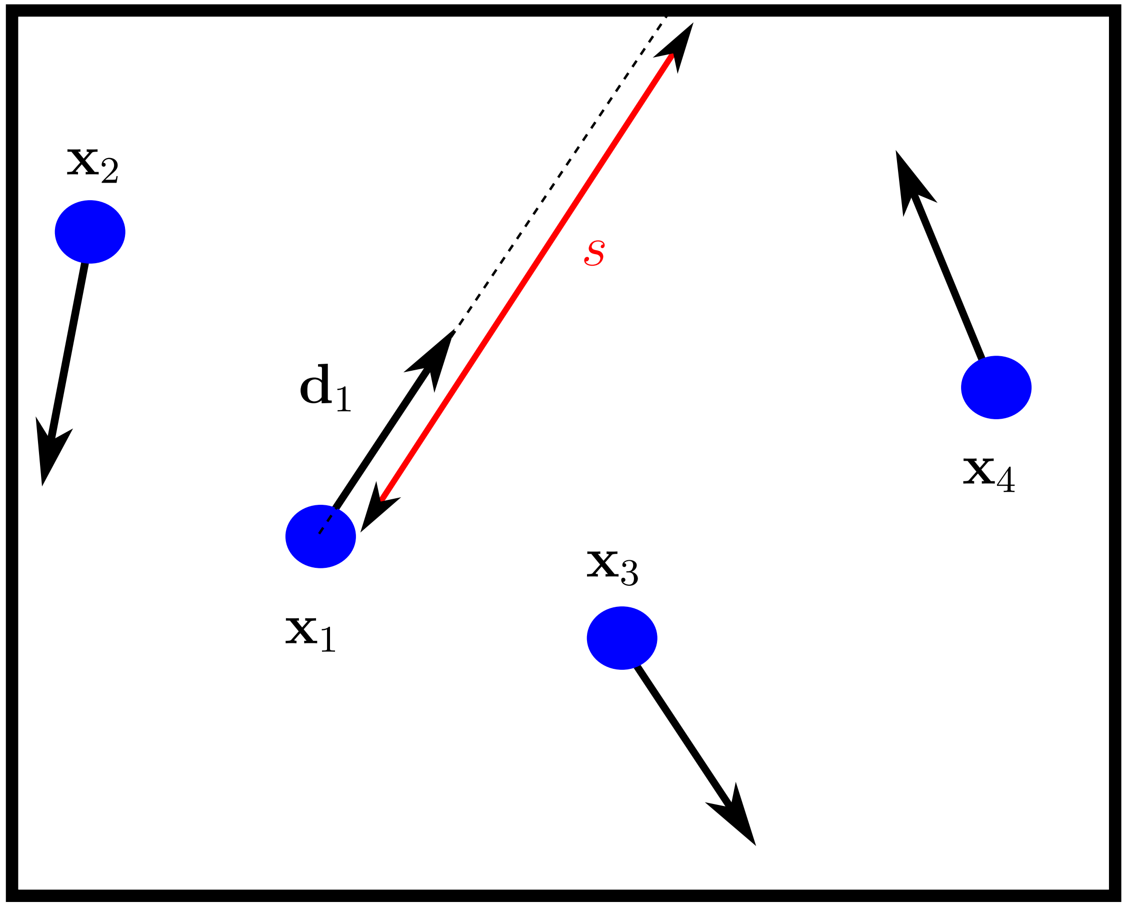

vector of particles

- what can we **gain** from this, assuming that we manage to have vector of particles in the first place?

Reminder: Data Parallelism and SIMD instructions

- **why do we hope to gain from vector processing?**

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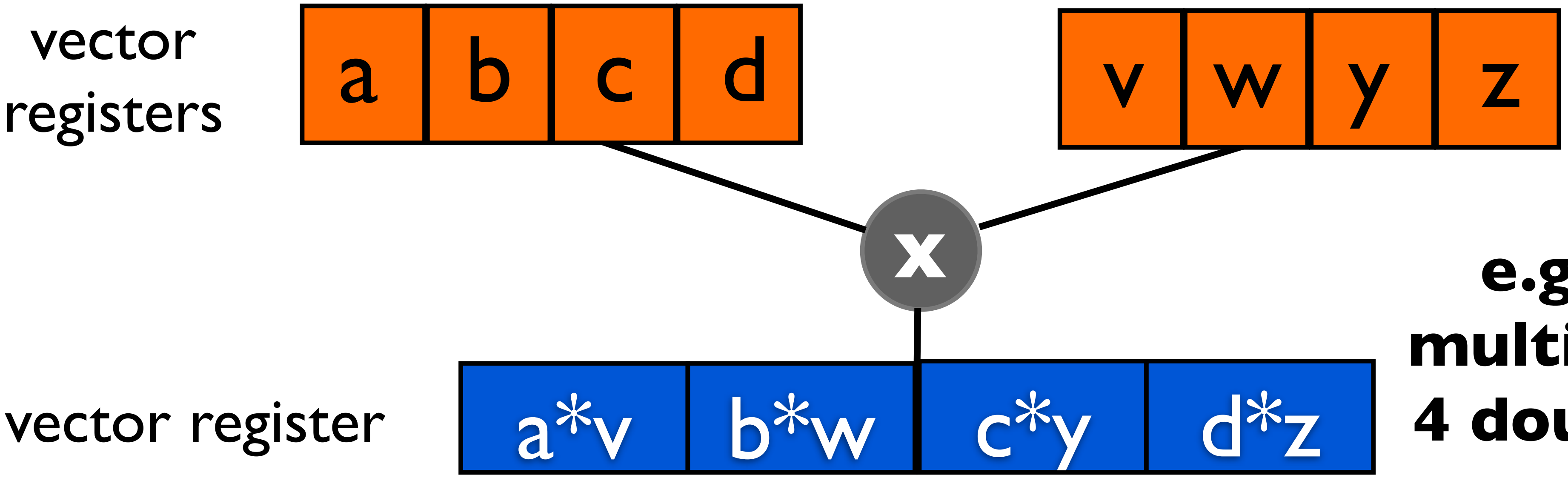
- “vectorized data” is a prerequisite to make efficient use of modern CPU vector instruction sets (“microparallelization”)



e.g., parallel multiplication of 4 doubles (AVX)

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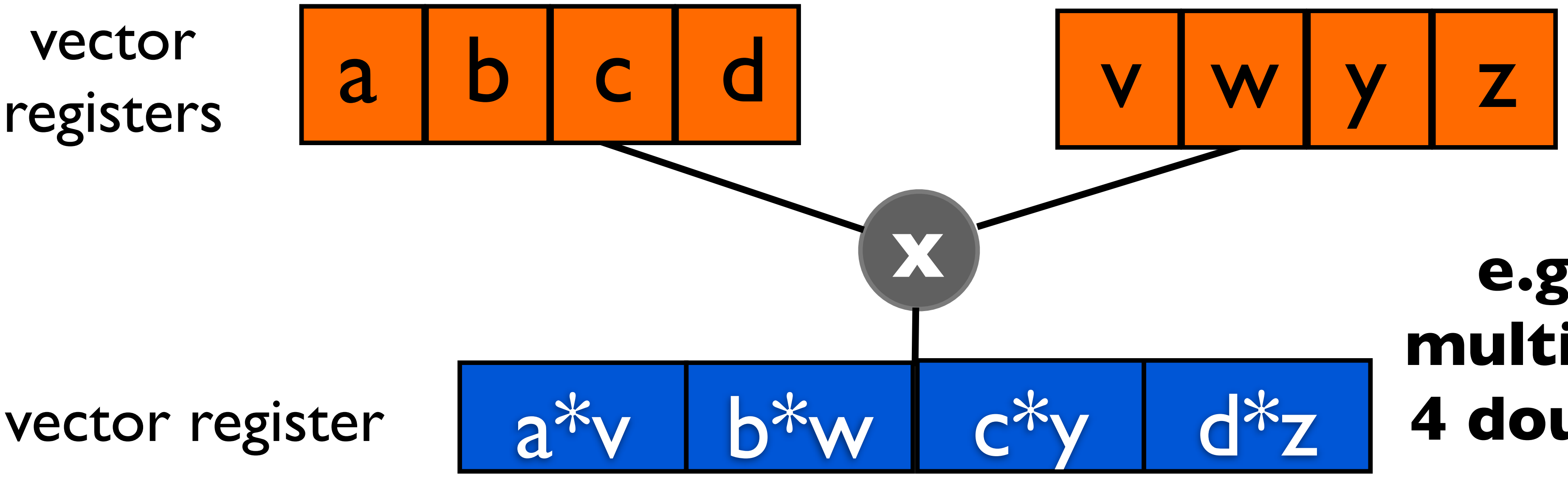

e.g., parallel multiplication of 4 doubles (AVX)

- effective use of vector instruction essential in order to make full use of current CPUs

- if we can gain from SIMD instructions, code is also **better prepared for accelerators** (GPUs, Intel Phi, ...)

Demonstrator Goals

Primary Goals

- setup simple vectorized geometry "demonstrator" to gain **development experience** and to **evaluate possible gains/pitfalls**
- focus for now on **CPU SIMD** opportunities (AVX instructions)
- vector optimize 3 geometries/shapes from simple to hard
  - **TGeoBBox**, TGeoCone, TGeoPolyCone
  - starting with TGeoBBox as most elementary block (needed also by more complicated shapes)

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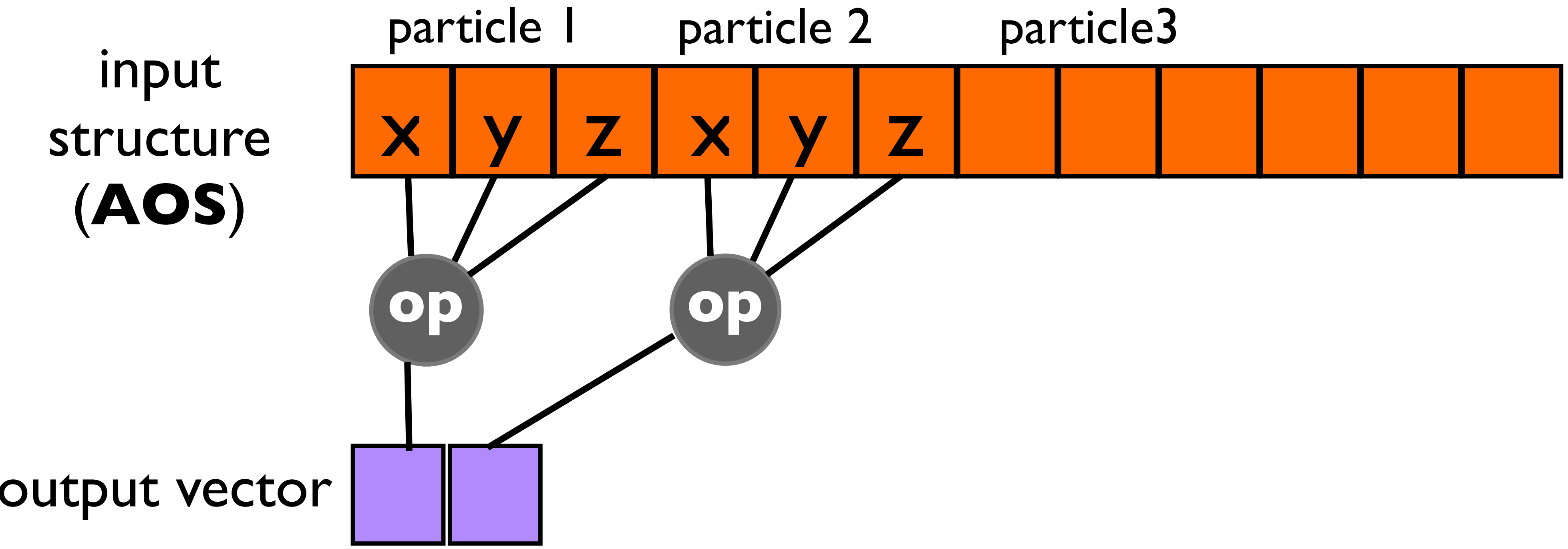
Requirements (wishes)

- rely on **existing code** base for geometry (here ROOT / USolid geometry)
- target compiler **autovectorization** whenever possible (in contrast to programming in intrinsics or some wrapper)
- compiler/platform **independence** ????

Some general things to fight with

- refactoring code to make use of SIMD instructions can be a major undertaking ... (see next slides)
- unfortunately **considerable differences** between compilers ... bad when trying to develop generic code
- **Intel icc (v13)** generally better than **gcc/4.8**
  - but often only with the help of **“forcing” pragmas** (#pragma ivdep, #pragma simd)
- a particular difference seems to be vector element access patterns...

Memory Access Problem / Consideration



- a natural way to do vector processing of particles would be AOS approach
- above memory access pattern typical (3-to-1)
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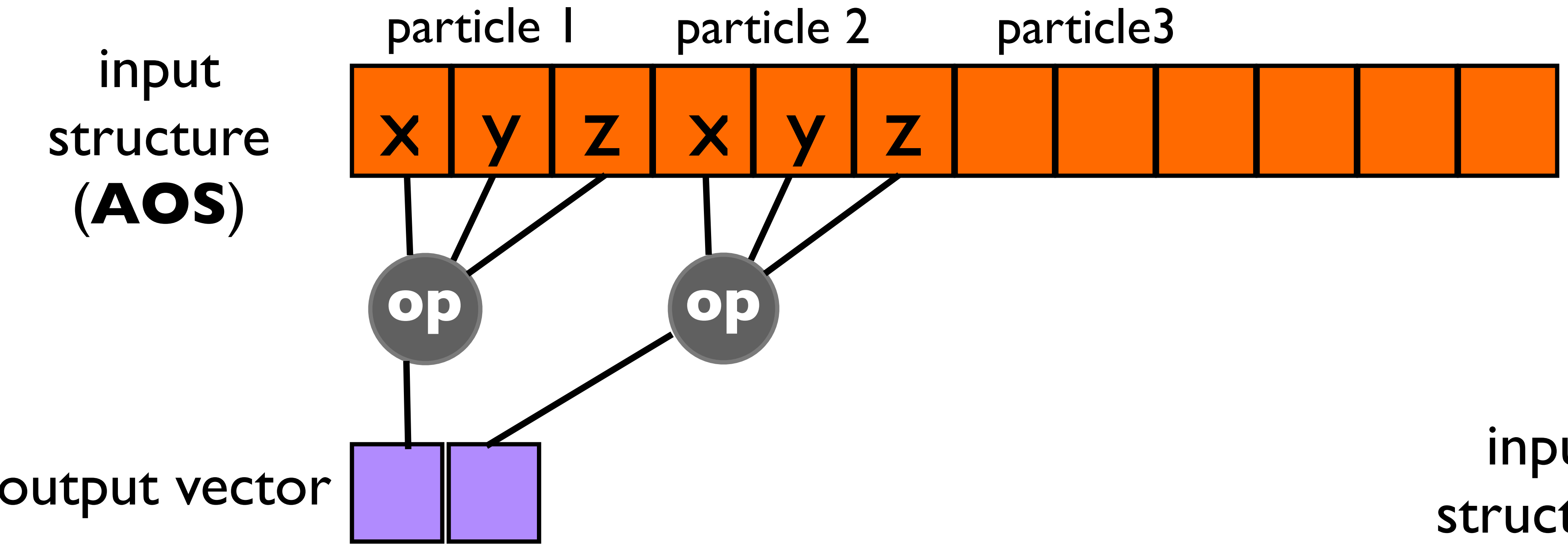

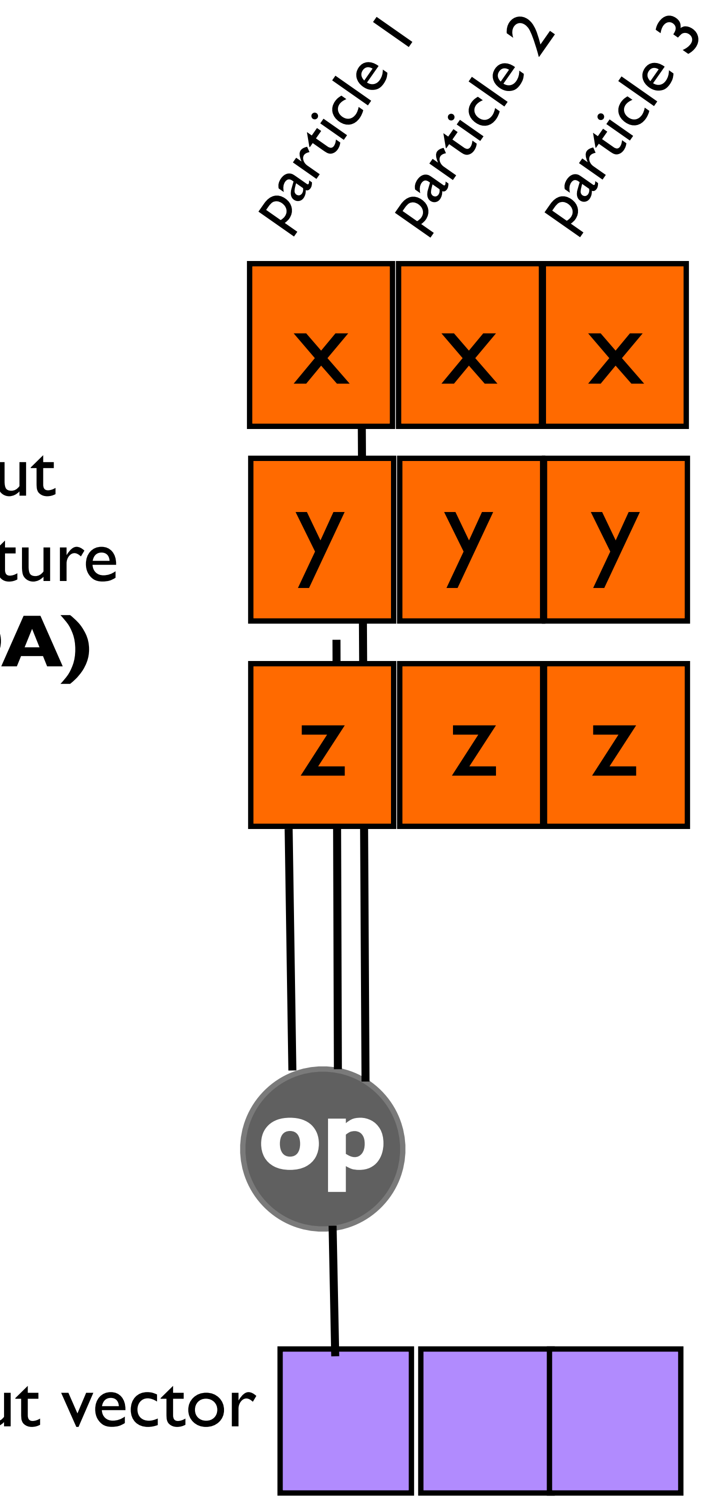

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- SOA approach is better autovectorizable
- memory access in SOA pattern also more efficient

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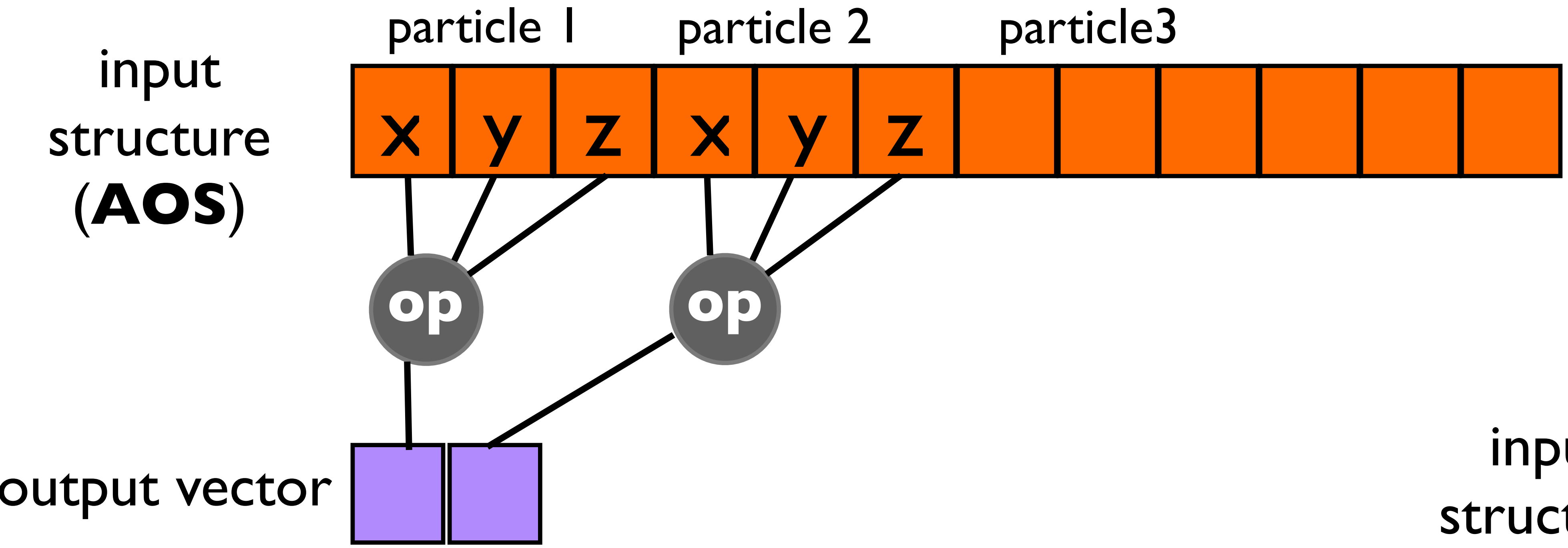

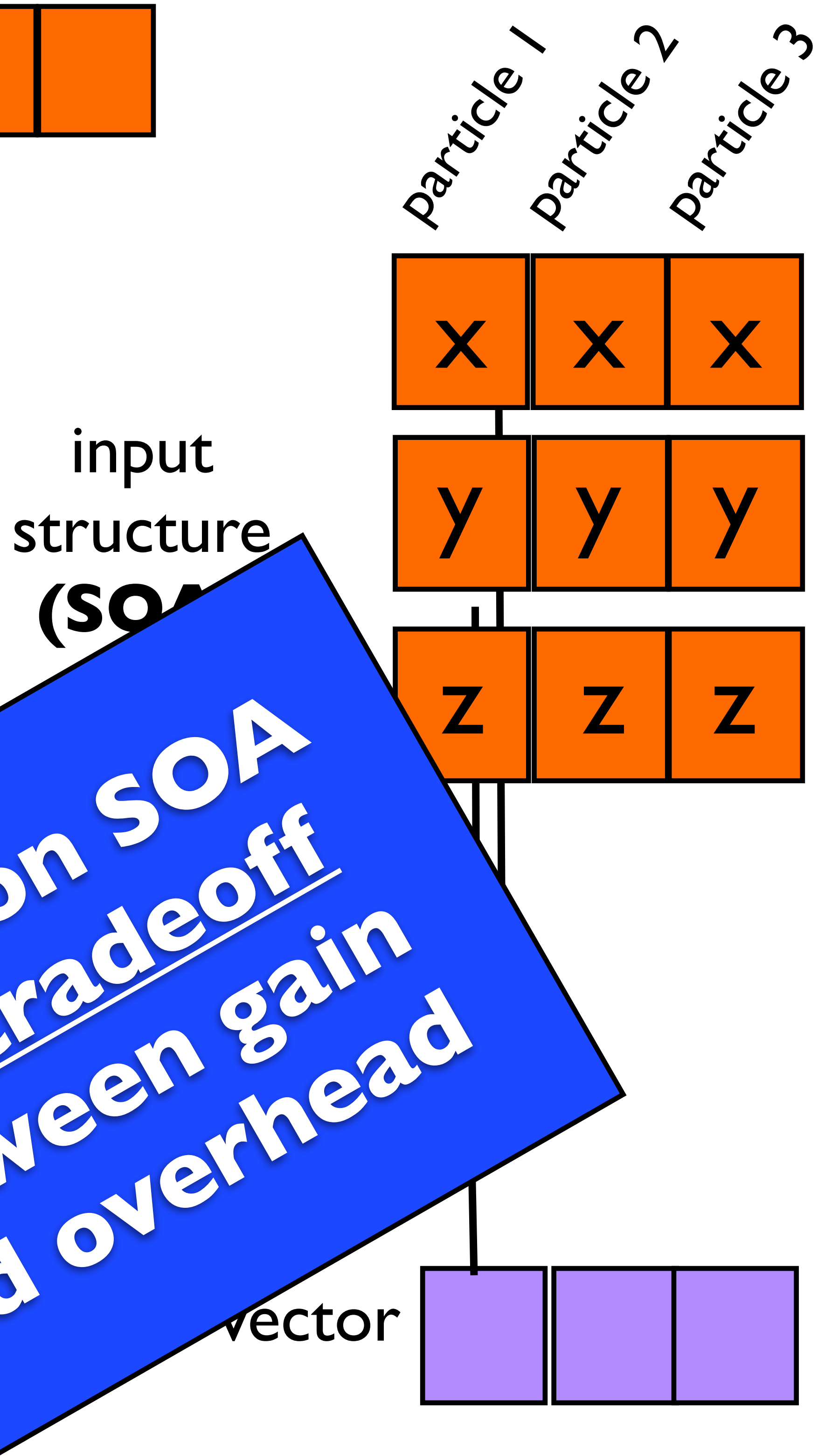

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Focus on SOA but tradeoff between gain and overhead

Hurdles on the way to (auto)vectorization

- **starting point: some existing code** (here easy example)

```
bool contains( const double * point ){
    for( unsigned int dir=0; dir < 3; ++dir ){
        if( fabs (point[dir]-origin[dir]) > boxsize[dir] )
        return false;
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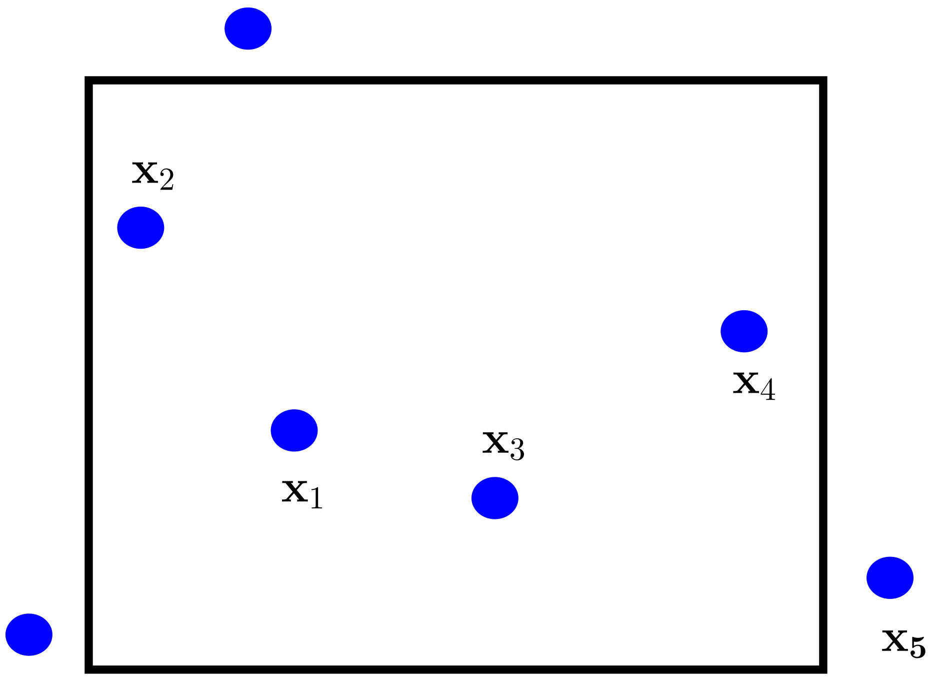

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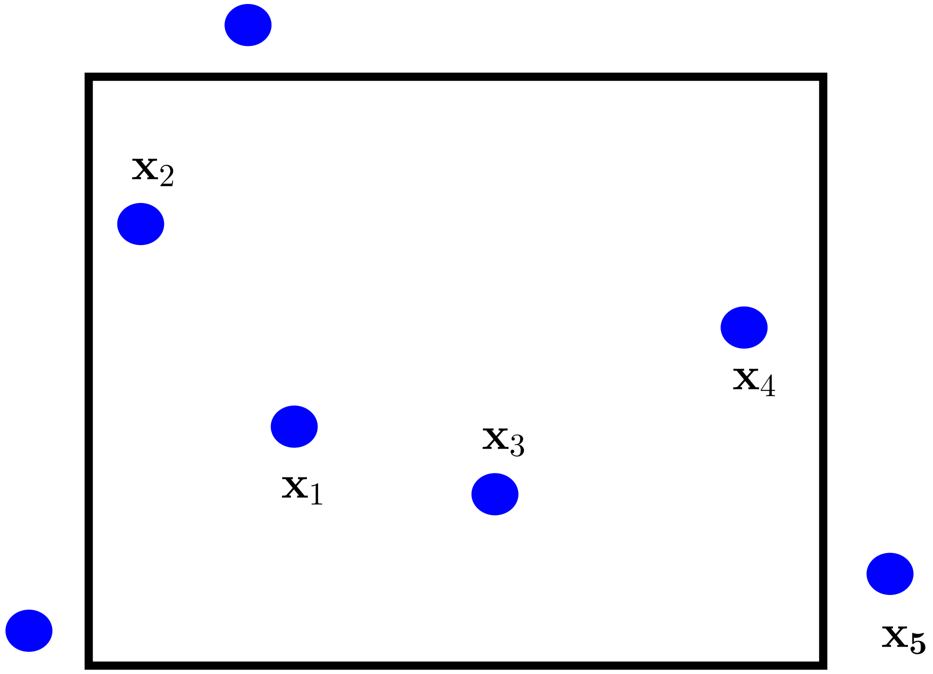

- **step 0: provide vector-interface**, call basic/elemental function ... and hope that compiler autovectorizes ...

```
void contains_v( const double * point, bool * isin, int np ) {
    for( unsigned int k=0; k < np; ++k) {
        isin[k]=contains( &point[3*k] );
}}
```

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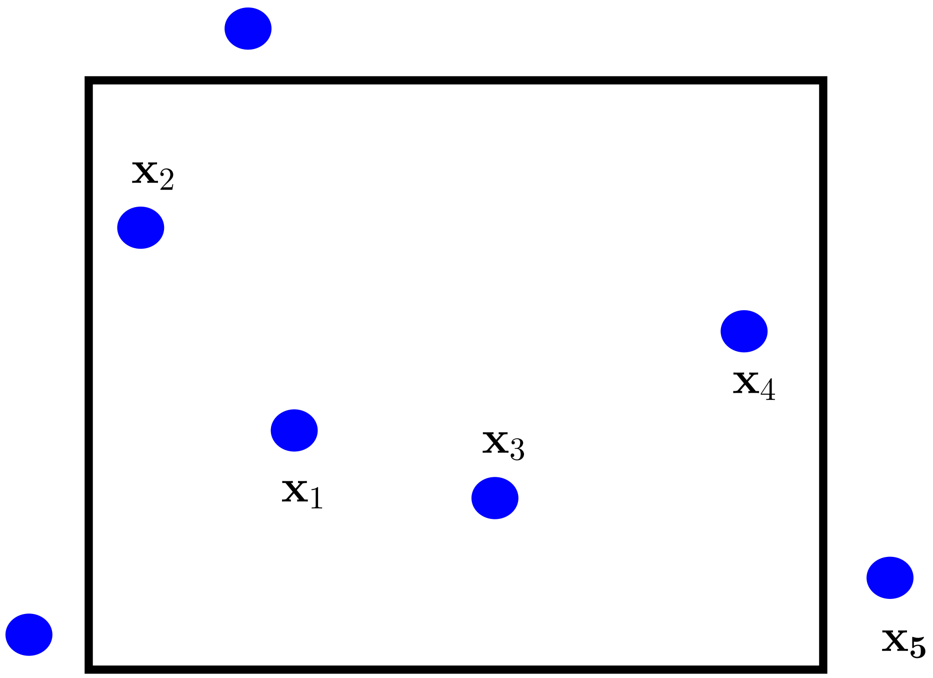

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```

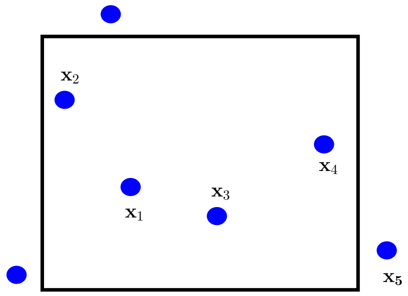
no auto-vectorization*

*icc: #pragma simd ok

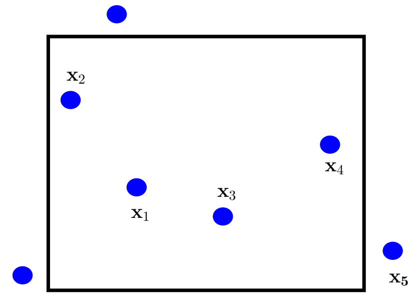
Hurdles on the way to (auto)vectorization (2)

- **step 1: inline and remove early returns**

```
void contains_v3( const double * point, bool * isin, int np ){
  for( unsigned int k=0; k < np; ++k){
     for( unsigned int dir=0; dir < 3; ++dir ){
     if ( fabs ( point[3*k+dir]-origin[dir] ) > boxsize[dir] ) isin[k]=false;
    }
    isin[k]=true;
}}
```



Hurdles on the way to (auto)vectorization (2)



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```

step 2: intermediate local variables + if conversion

```
 void contains_v4( const double * point, bool * isin, int np){
  for( unsigned int k=0; k < np; ++k){
     bool tmp[3]={true, true, true};
     for( unsigned int dir=0; dir < 3; ++dir ){
      tmp[dir] = fabs ( point[3*k+dir]-origin[dir] ) > boxsize[dir]; }
      isin[k]=tmp[0] & tmp[1] & tmp[2];
 }}
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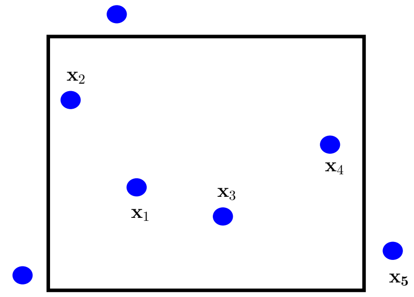

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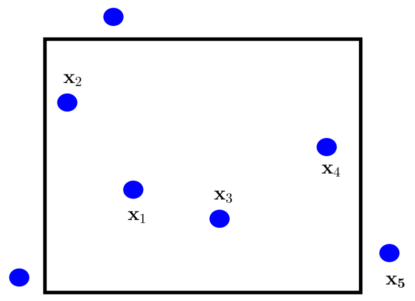
*icc: #pragma ivdep ok

Hurdles on the way to (auto) vectorization (3)

- **step 3: AOS - SOA conversion**



```
 typedef struct {
   double *coord[3];
 } P;

void contains_v6( const P &  point, bool * isin, int np ){
  for( unsigned int k=0; k < np; ++k){
      bool tmp[3];
      for( unsigned int dir=0; dir < 3; ++dir ){
        tmp[dir] = (fabs (point.coord[dir][k]-origin[dir]) > boxsize[dir]);
     }
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Hurdles on the way to (auto) vectorization (3)

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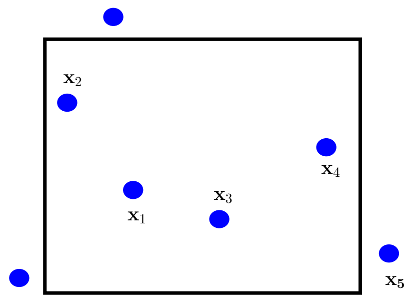

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*gcc/4.7 ok ?? , gcc/4.8 no

Hurdles on the way to (auto)vectorization (4)

- **step 4: (manually) unroll inner loops in source**

```
void contains_v7( const P & points, bool *  isin, int np ){
  for( unsigned int k=0; k < np; ++k)
  {
      bool resultx=(fabs (point.coord[0][k]-origin[0]) > boxsize[0]);
      bool resulty=(fabs (point.coord[1][k]-origin[1]) > boxsize[1]);
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}}
```

this auto-vectorizes !!

- **this is only version** that **autovectorizes uncondionally** with all compilers tested (icc 13, gcc 4.7/4.8)

- to arrive here, **needed ca. 4 refactoring steps**

many methods are MUCH!! more complicated

- (shortened) example from TGeoPCon:: DistFromOutside

```
double TGeoPcon::DistFromOutside(double *point, double *dir, double step){
    /// ....
    double r2 = point[0]*point[0]+point[1]*point[1];
    double radmax=0;
    radmax=fRmax[TMath::LocMax(fNz, fRmax)];
    if (r2>(radmax*radmax)) {
        double rpr=-point[0]*dir[0]-point[1]*dir[1];
        double nxy=dir[0]*dir[0]+dir[1]*dir[1];
        if (rpr<sqrt((r2-radmax*radmax)*nxy)) return TGeoShape::Big();
    }
    int ipl = TMath::BinarySearch(fNz, fZ, point[2]);
    int ifirst = ipl;
    if (ifirst<0) {
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    } else if (ifirst>=(fNz-1)) ifirst=fNz-2;
    // compute distance to boundary
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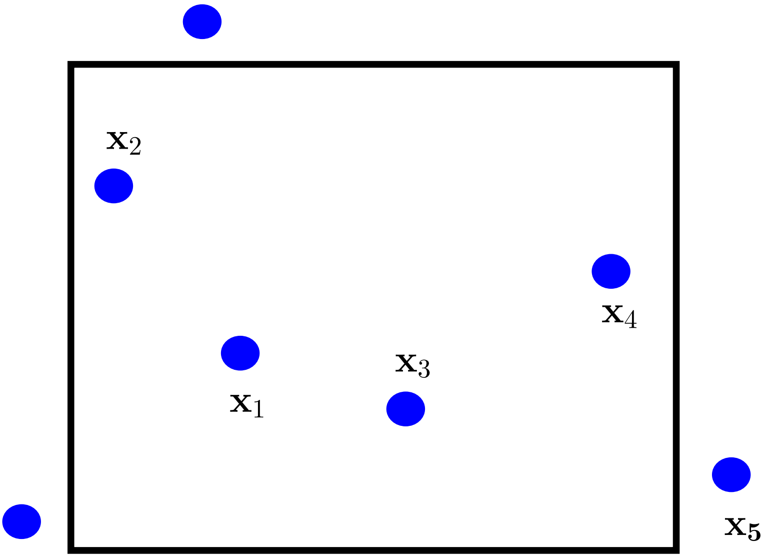
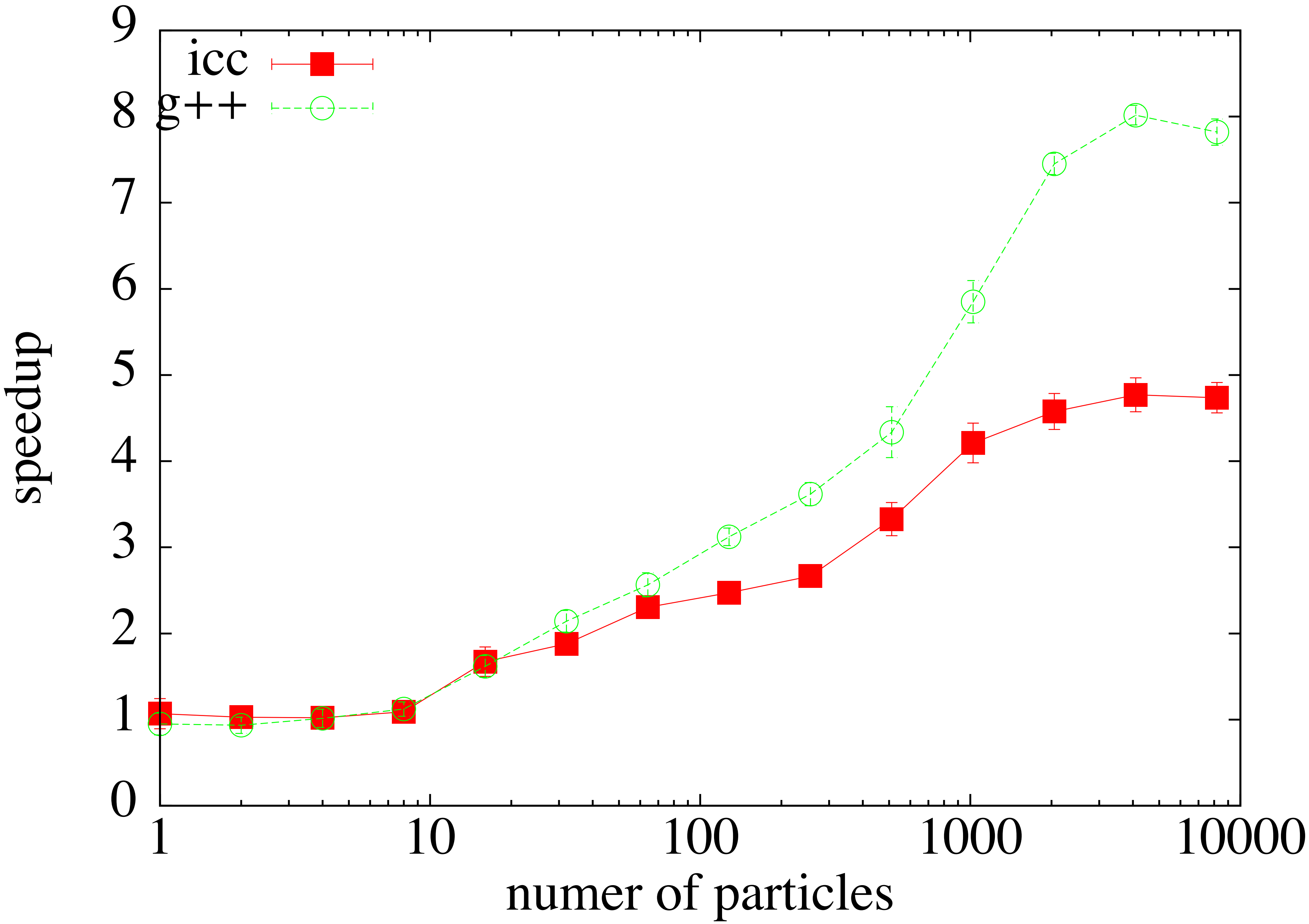
- we may be satisfied with **partial vectorization** (e.g., of expensive math functions)

First Performance Evaluation
-- Status for TGeoBBox --

TGeoBBox Performance Evaluation: Contains

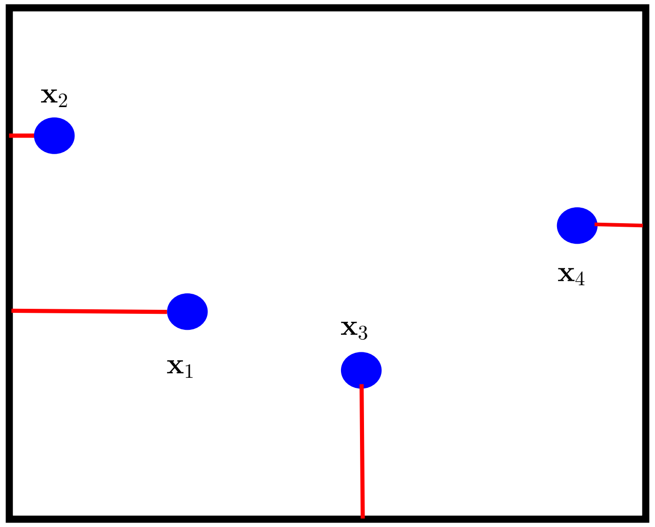
- calculates if particle inside box (see slides above)
- status: **both gcc/icc autovectorize, very good speedup**
- Intel iCore7 / AVX instructions

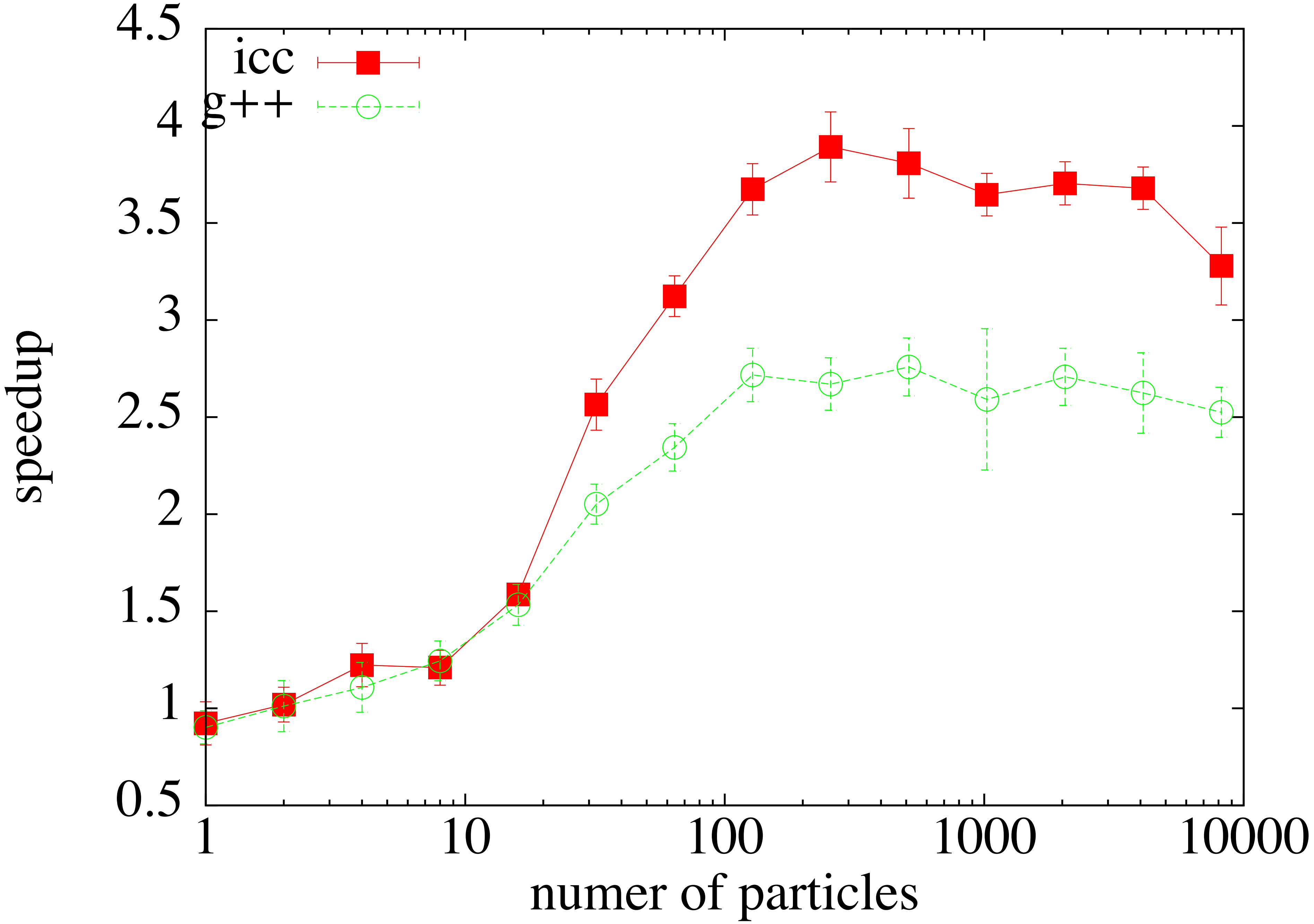




TGeoBBox Performance Evaluation: GetSafety

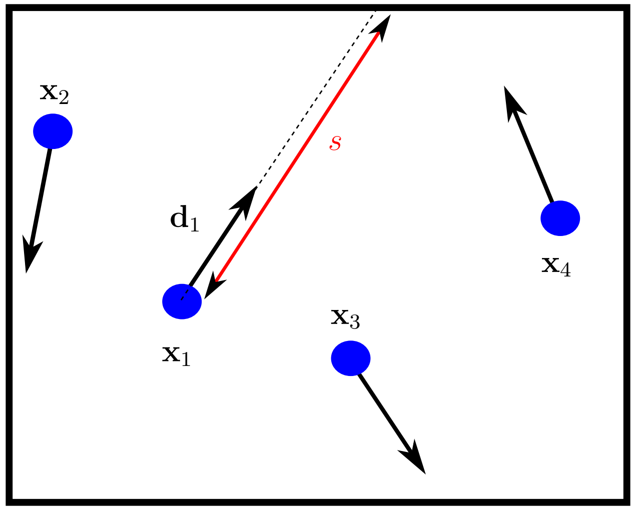
- calculates minimum distance to any surface
- status: **both gcc/icc autovectorize, good speedup**
- Intel iCore7 / AVX instructions

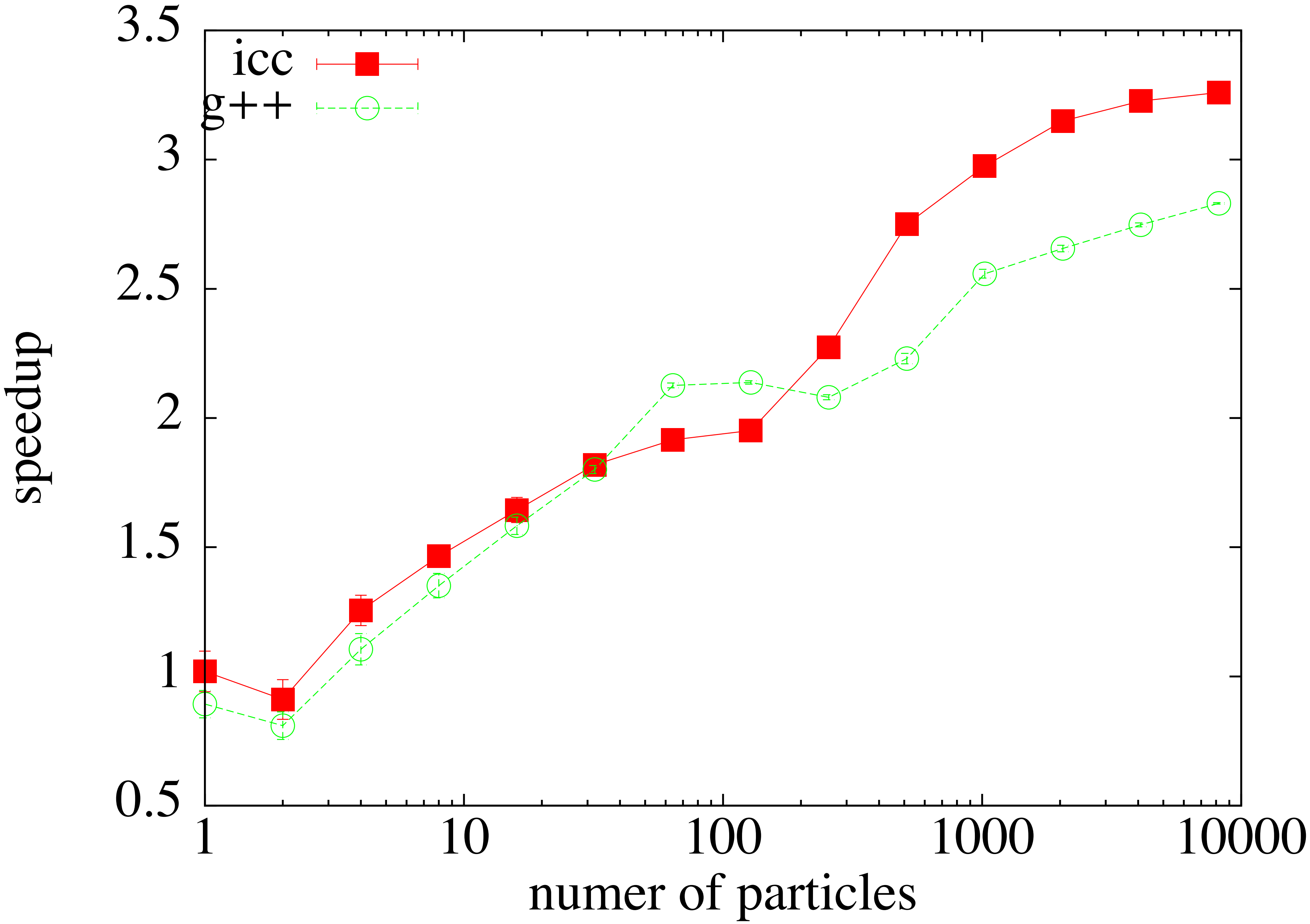




TGeoBBox Performance Evaluation: DistFromIn

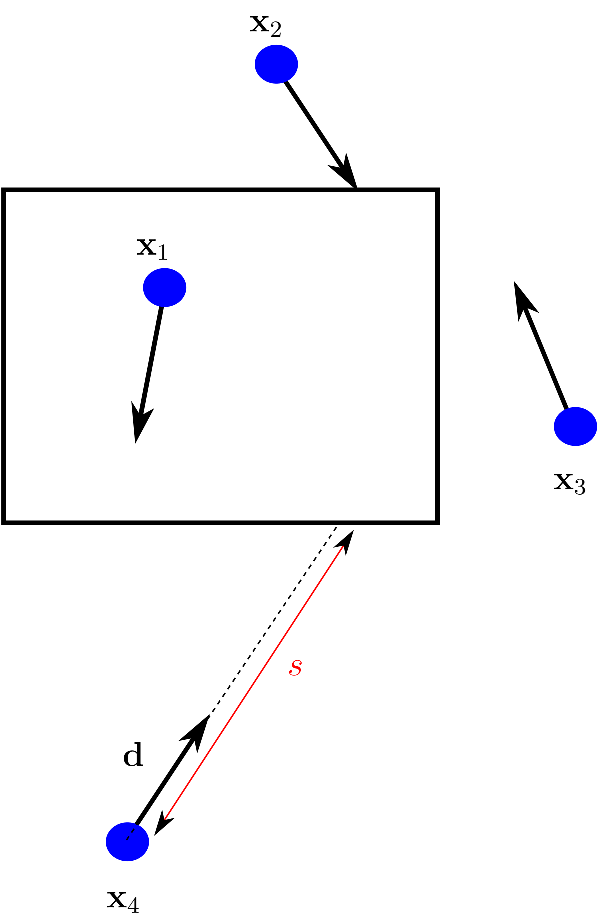
- calculates distance to hitting surface from inside
- status: **both gcc/icc autovectorize, good speedup**

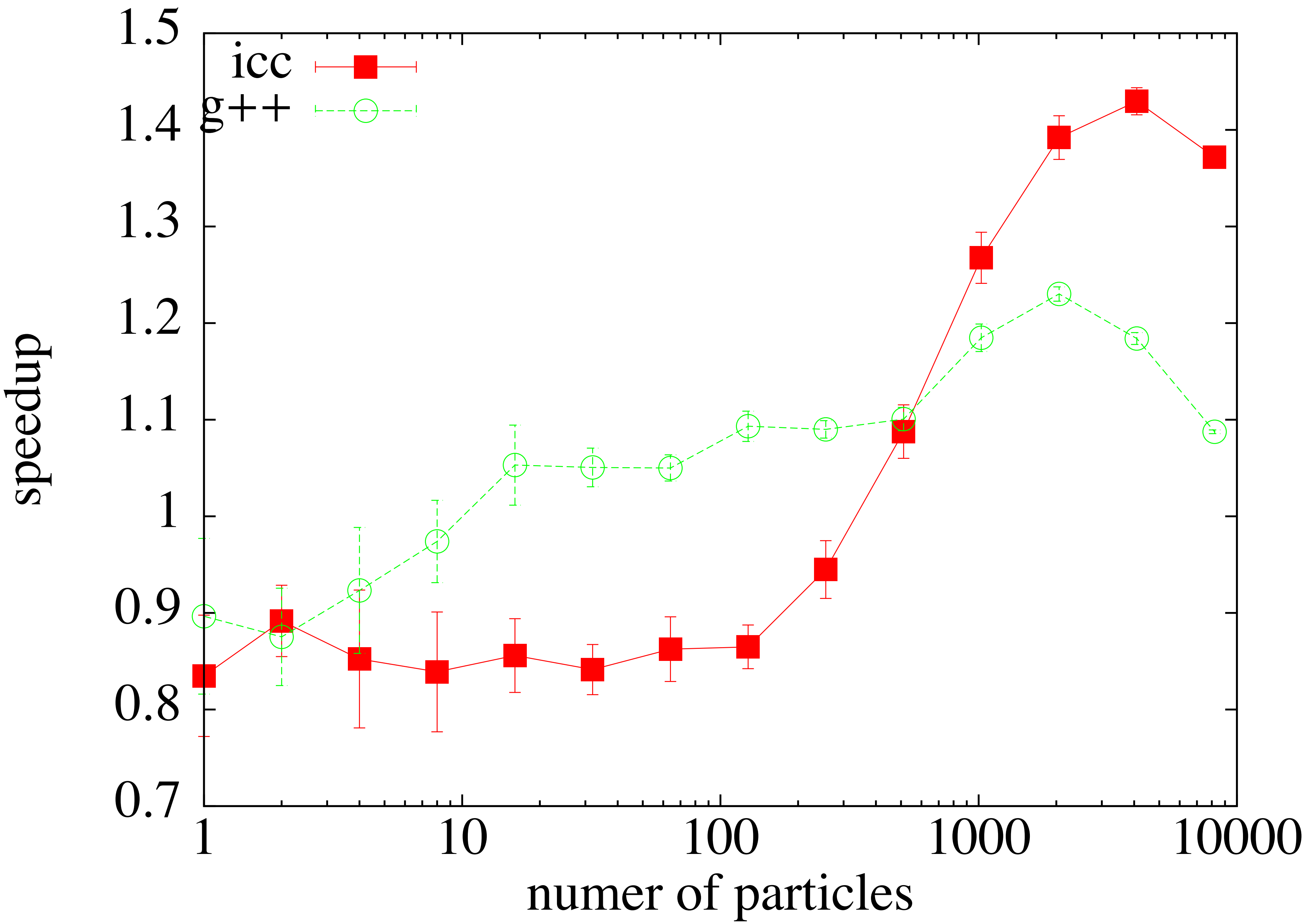




Performance Evaluation: DistFromOut

- calculates distance to hitting surface from outside
- status: **only icc autovectorizes** (too many conditionals??)
- initial performance **penalty** for small vectors (due to early return removals), some gain for larger number of particles





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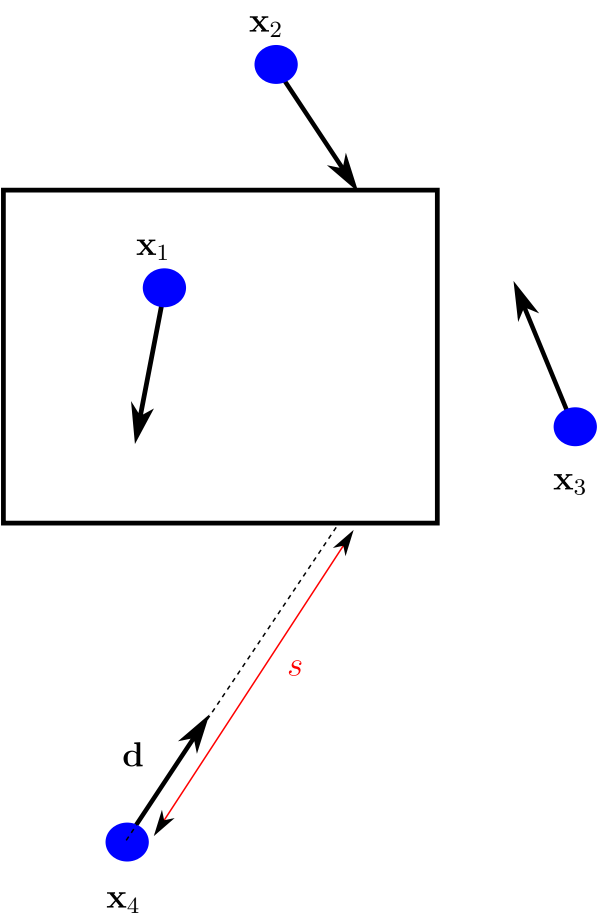

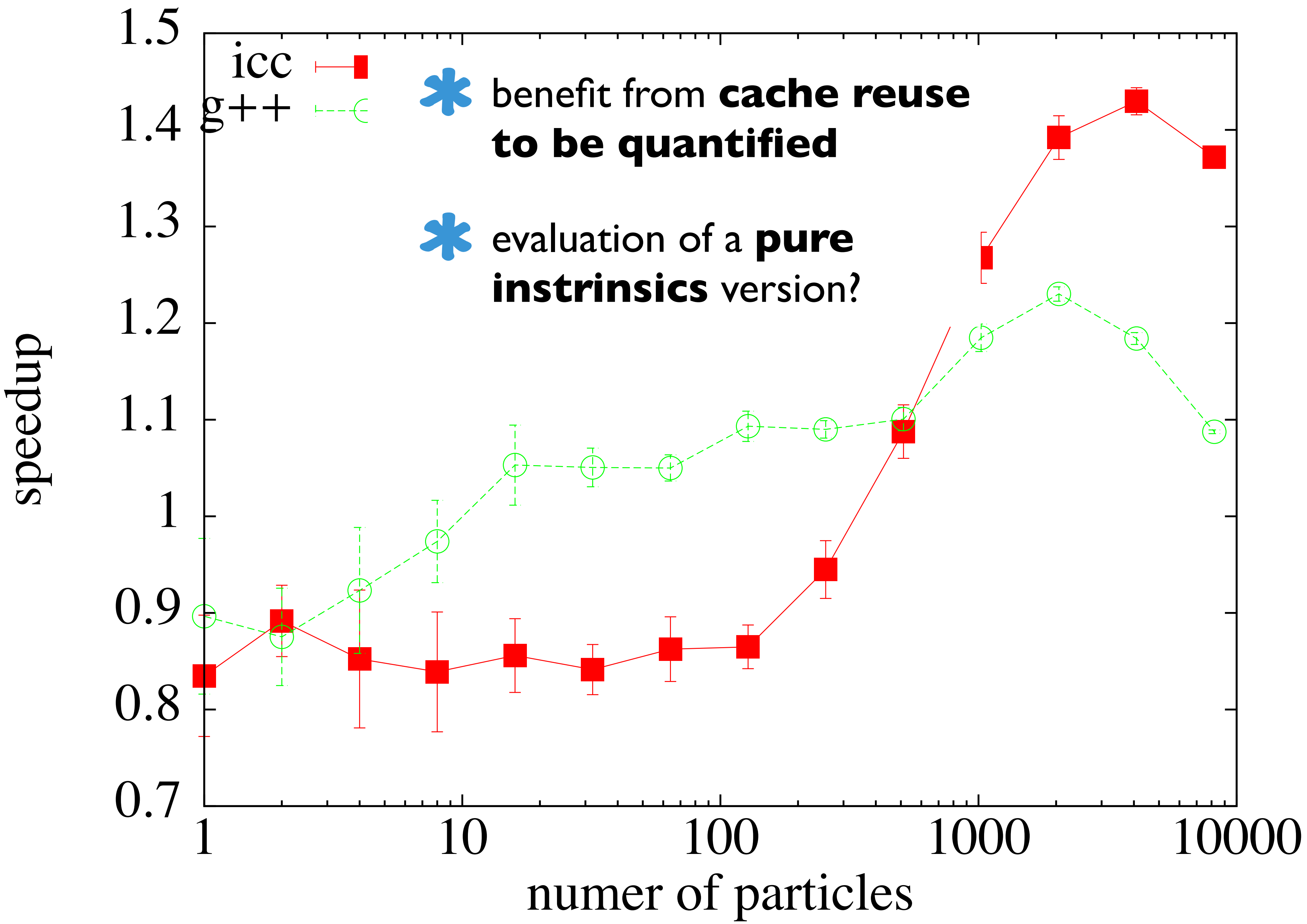

- benefit from **cache reuse to be quantified**
- evaluation of a **pure instrinsics** version?

Summary / Outlook

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- talked about challenges in optimizing geometry routines for “vector particle processing”
- rather expensive work-process, complete code rewrite often unavoidable
- on average good SIMD performance results for TGeoBBox methods
- for more complex shapes to be seen ... hope to gain at least from better cache performance

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Outlook

- more complex shapes
- GPUs, Xeon Phi
- evaluate **performance gains from cache reuse**
- quantification of SOA conversion overhead

Backup: A need for tools...

- converting code for data parallelism can be a pain ... (see challenges)
- would be nice to have better tool support for this task, helping at least with often recurring work

A possible direction:

- **source-to-source transformations** (preprocessing)
  - provide trivial vectorized code version of a function
  - unroll inner loops, rewrite early returns, ...
  - Clang/LLVM API very promising for this ... currently investigating

LLVM COMPILER INFRASTRUCTURE

- some tools go into this direction:
  - Scout (TU Dresden): Can take code within a loop and **emit instrinsics** code for all kinds of architectures
  - could be used in situations where the compiler does not autovectorize

SCOUT A Source-to-Source Transformator for SIMD-Optimizations

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Stay tuned !!

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