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FORSCHUNGSZENTRUM

Accelerating Plasma Physics with GPUs

PADC Annual Workshop 2016

Andreas Herten, Forschungszentrum Jülich, 17 October 2016

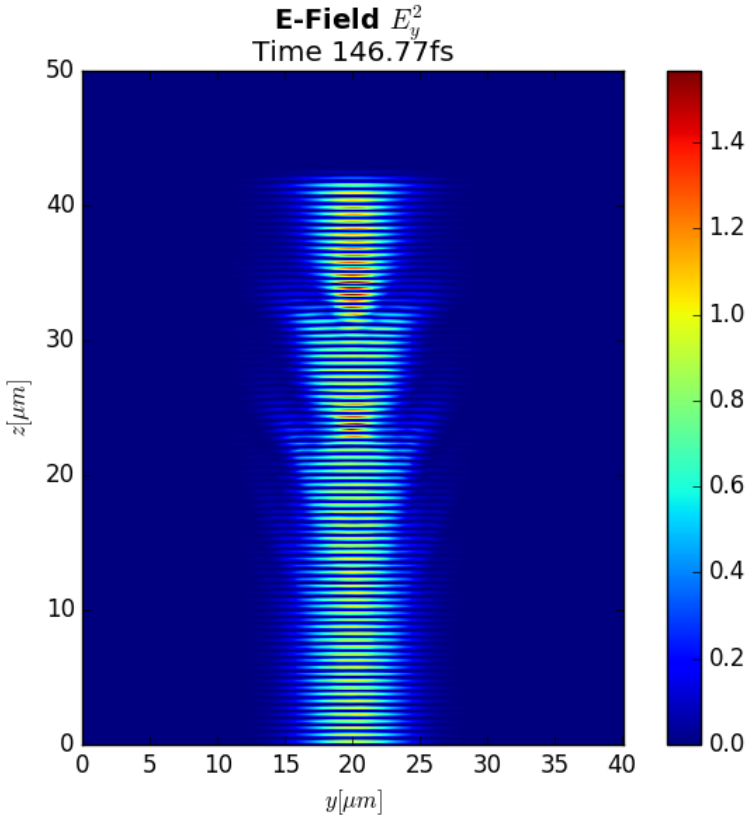
Contents

- JuSPIC on GPU
- With OpenACC
- Not with OpenACC
- Performance Model

JuSPIC: Introduction

man juspic

- **JuSPIC**: Jülich Scalable Particle-in-Cell Code
- Based on PSC by H. Ruhl
- Developed at JSC by SimLab Plasma Physics
- 3D electromagnetic Particle-in-Cell
- Properties
  - Solves relat. Vlasov equations, Maxwell equations
  - Scheme: Finite-difference time-domain
  - Cartesian geometry
  - Arbitrary number of particle species



JuSPIC: Technologies

A quite parallel code

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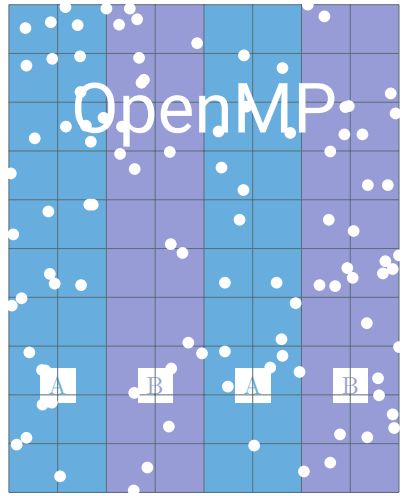
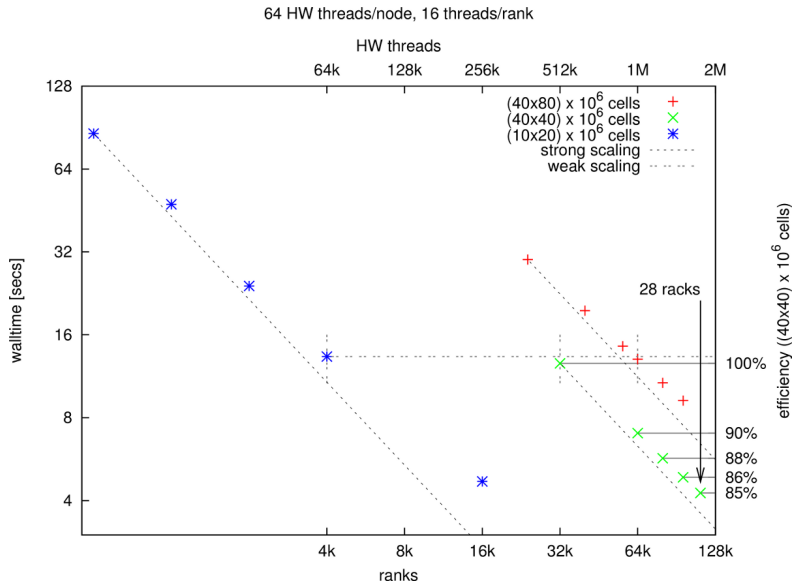
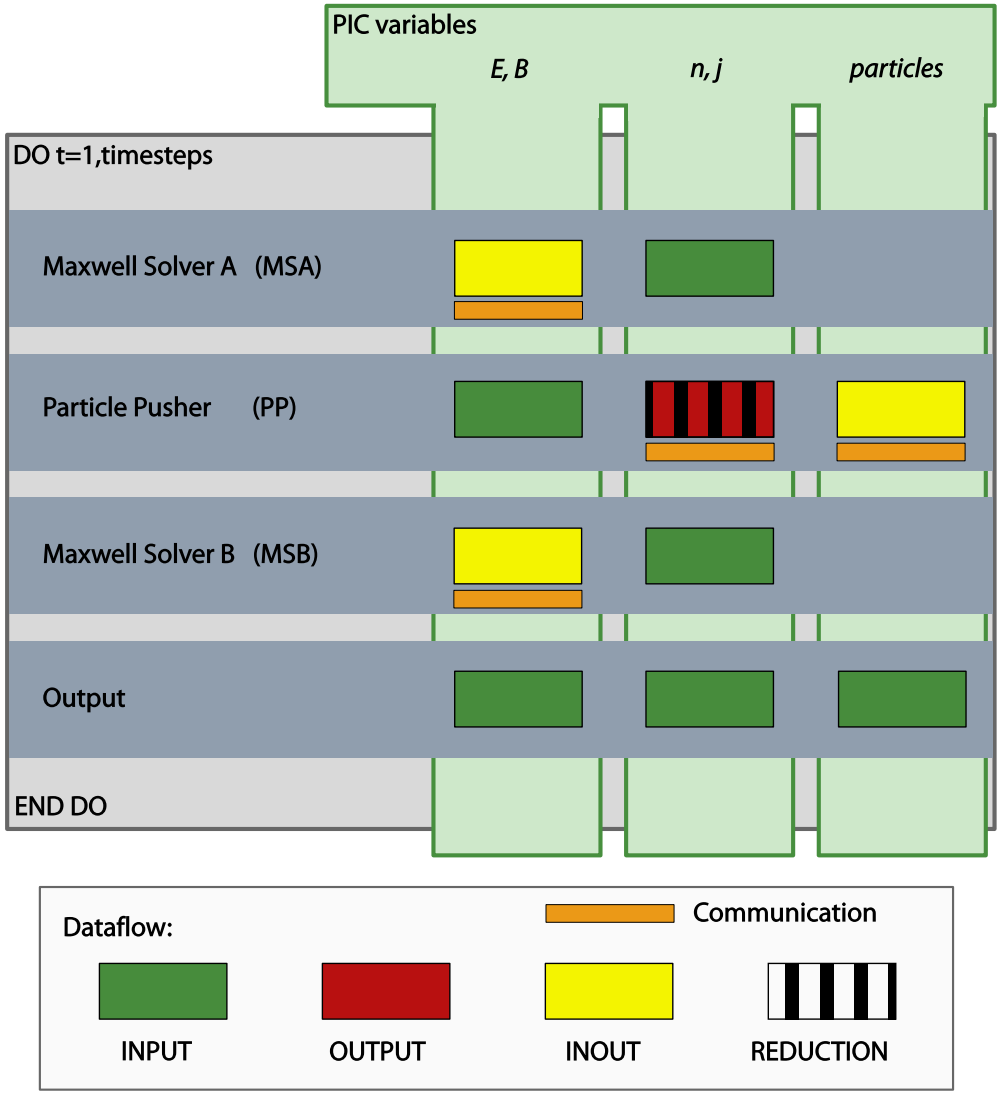
- Modern Fortran
- Distributed with **MPI**
  Domain decomposition: 3D
- CPU-parallelized with **OpenMP**
  Domain decomposition: Slices
- Particles connected by linked list
- High-Q Club:
  Scales to full JUQUEEN





Stages of Program



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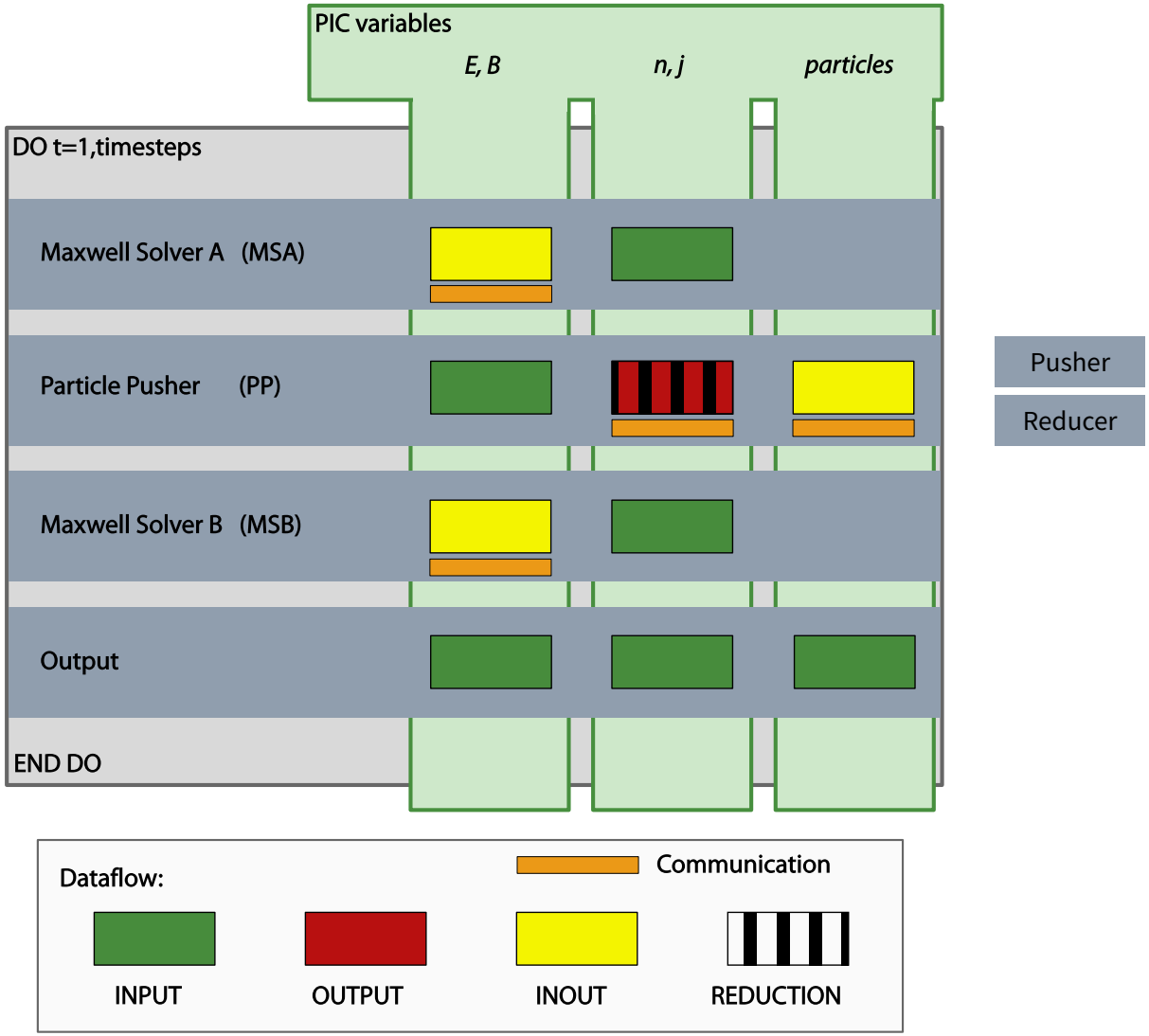

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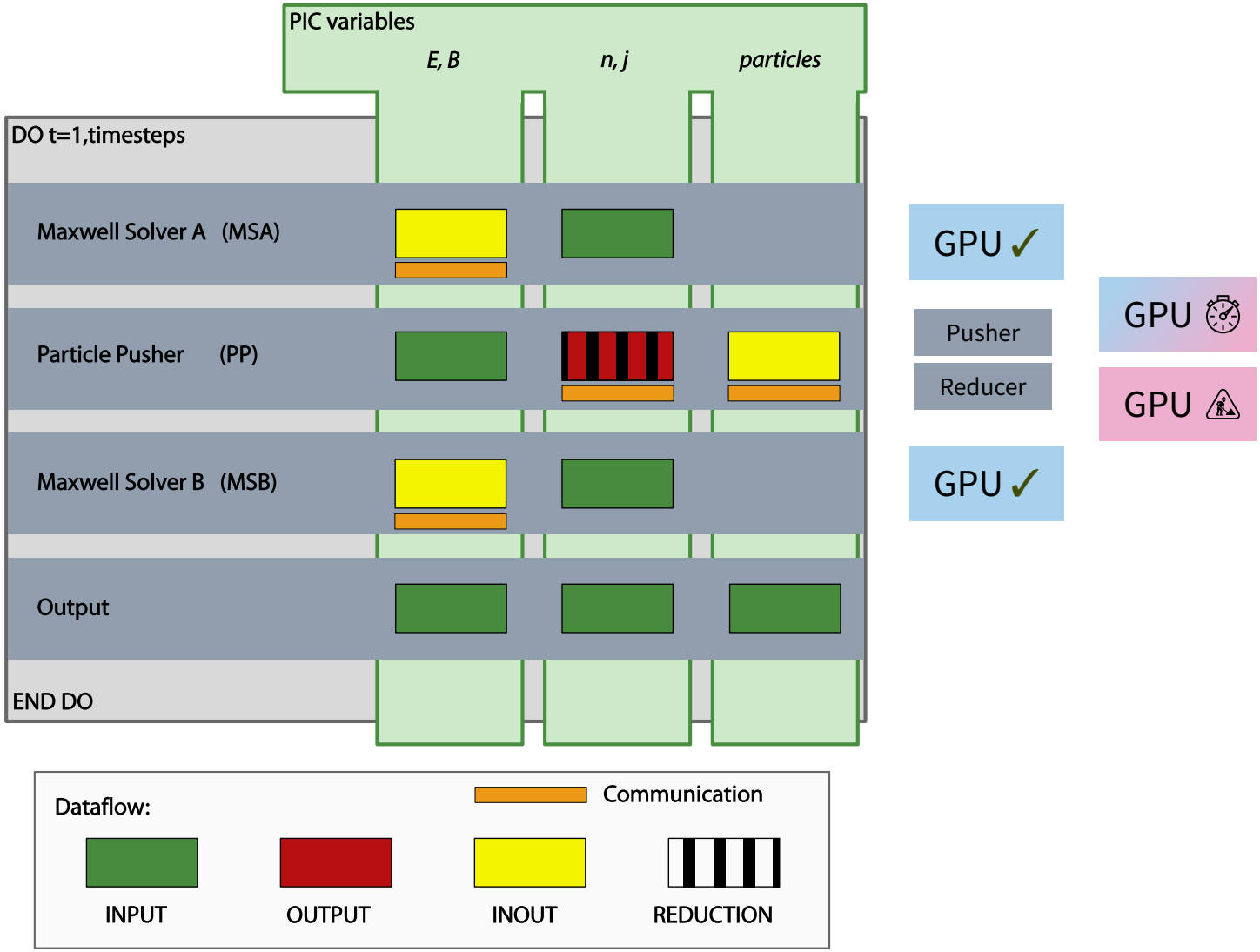

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Acceleration

Accelerating JuSPIC

Start of the journey

JÜLICH FORSCHUNGSZENTRUM

- *Initial* requirements
  - Leverage parallelism offered by GPUs
  - Still work on all platforms
  - Optimizations not solely for GPUs
  - → **OpenACC**

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OpenACC:

- Many cores with `pragmas`
- *(Not)* like OpenMP
- NVIDIA, AMD, …
- PGI, Cray, GCC
- C, Fortran

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- Profiling
  1. Particle Reducer (64 %)
  2. Particle Pusher (32 %)
  3. Maxwell Solver (1 %)

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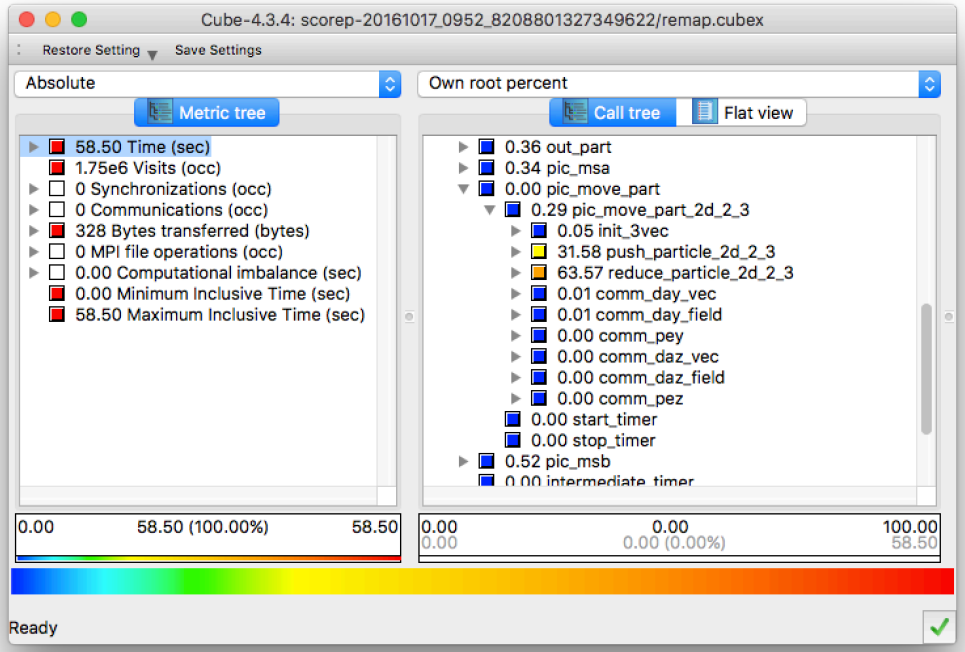

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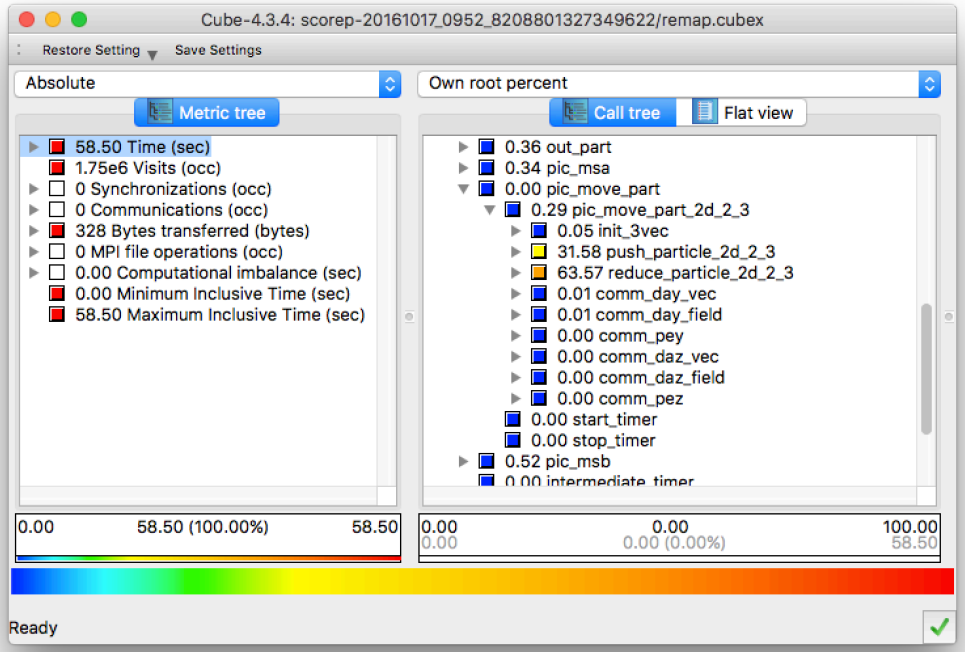

Maxwell Solver

Straight forward

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- Content of function: Update $\vec{E}$ and $\vec{B}$ fields
- Global data handling
- Source example

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```
!
do i3=i3mn-1,i3mx+1
  do i2=i2mn-1,i2mx+1
    do i1=i1mn-1,i1mx+1
      e(i1,i2,i3)%X=e(i1,i2,i3)%X  +
      ↪  cny*(b(i1,i2,i3)%Z-b(i1,i2-1,i3)%Z) -
      ↪  cnz*(b(i1,i2,i3)%Y-b(i1,i2,i3-1)%Y) -
      ↪  0.5*dt*ji(i1,i2,i3)%X
      ! ...
```

Maxwell Solver

Straight forward

- Content of function: Update $\vec{E}$ and $\vec{B}$ fields
- Global data handling
- Source example

```
!$acc kernels loop collapse(3) present(e,b,ji)
do i3=i3mn-1,i3mx+1
  do i2=i2mn-1,i2mx+1
    do i1=i1mn-1,i1mx+1
      e(i1,i2,i3)%X=e(i1,i2,i3)%X  +
      ↪  cny*(b(i1,i2,i3)%Z-b(i1,i2-1,i3)%Z) -
      ↪  cnz*(b(i1,i2,i3)%Y-b(i1,i2,i3-1)%Y) -
      ↪  0.5*dt*ji(i1,i2,i3)%X
      ! ...
```

Maxwell Solver

Straight forward

- Content of function: Update $\vec{E}$ and $\vec{B}$ fields
- Global data handling

```
advance_e_vol:
  1410, Generating present(e(:,:,:),b(:,:,:),ji(:,:,:))
  1412, Loop is parallelizable
  1414, Loop is parallelizable
  1415, Loop is parallelizable
      Accelerator kernel generated
      Generating Tesla code
    1412, !$acc loop gang, vector(128) collapse(3) ! blockidx%x threadidx%x
    1414,   ! blockidx%x threadidx%x collapsed
    1415,   ! blockidx%x threadidx%x collapsed
```

```
                ↪   0.5*dt*ji(i1,i2,i3)%X
               ! ...
```

Maxwell Solver

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```

```
                ↪   0.5*dt*ji(i1,i2,i3)%X
               ! ...
```

Particle Pusher

Start of a journey…

- Content of function:
  Interpolate field, update particle position and momentum
- Change to source: Linked list of particles $\rightarrow$ array of particles

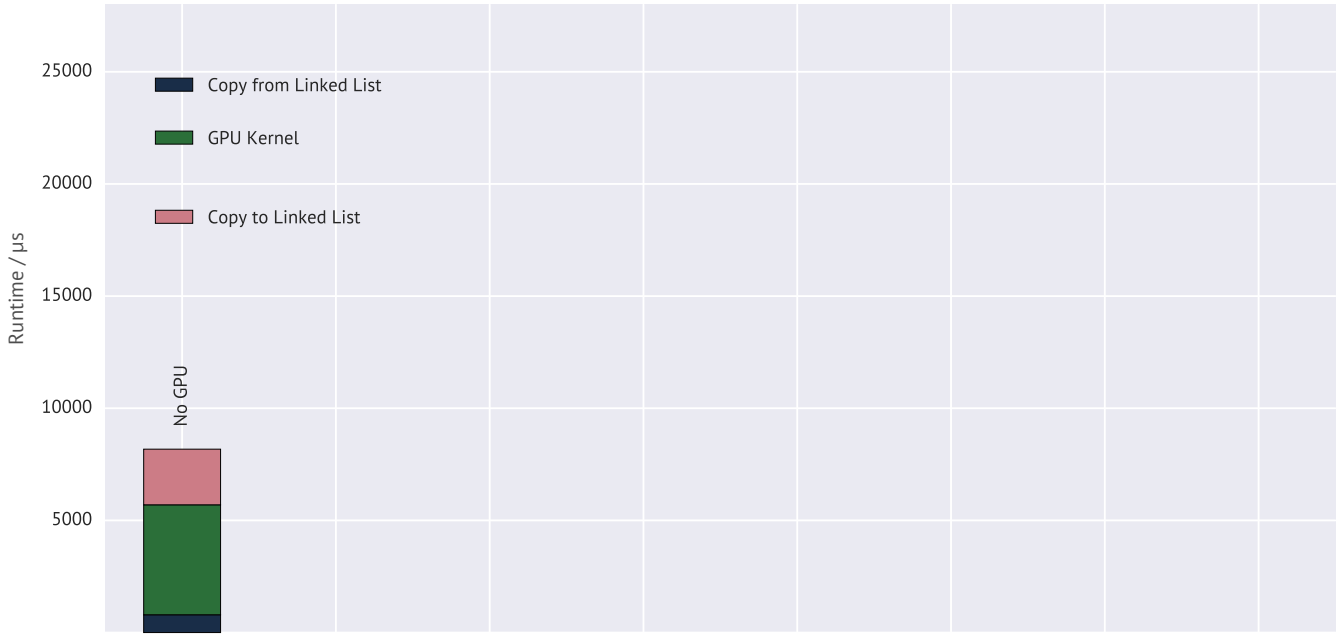
Particle Pusher

Start of a journey…

- Content of function:
  Interpolate field, update particle position and momentum
- Change to source: Linked list of particles $\rightarrow$ array of particles
- Timings

  ***CPU**: Intel Xeon Sandy Bridge (2 GHz), no MPI, no OpenMP*

  ***GPU**: NVIDIA Tesla K40, ECC enabled*



Acceleration with OpenACC

This should be easy, right?

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- Simple addition in front of code

```
do i_particle = loop_min, loop_max
   x_(:)=list_of_particles(i_particle)%vec(:)
   p_(:)=list_of_particles(i_particle)%pvec(:)
   qi   =list_of_particles(i_particle)%q

   mi=p_prop(list_of_particles(i_particle)%id)%m
   wi=p_prop(list_of_particles(i_particle)%id)%w

   root=1.0/sqrt(1.0+sum(p_**2))
   !...
```

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- Simple addition in front of code

```
!$acc parallel loop private(pp,root,qi,mi,wi) present(e,
↪  b) copy(list_of_particles)
do i_particle = loop_min, loop_max
   x_(:)=list_of_particles(i_particle)%vec(:)
   p_(:)=list_of_particles(i_particle)%pvec(:)
   qi   =list_of_particles(i_particle)%q

   mi=p_prop(list_of_particles(i_particle)%id)%m
   wi=p_prop(list_of_particles(i_particle)%id)%w

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```
!$acc parallel loop private(pp_root,qi,mi,wi) present(e,
```

```
push_particle_2d_2_3:
   875, include 'pic.in.gpu.minimallyunrolled.F90'
      254, Generating present(e(:,:,:),b(:,:,:))
         Generating copy(list_of_particles(:))
         Accelerator kernel generated
         Generating Tesla code
        255, !$acc loop gang, vector(128) ! blockidx%x threadidx%x
      254, Generating copyout(tvec3(:),tvec2(:),tvec1(:))
         Generating copyin(xyzl(2:),p_prop(list_of_particles%id))
         Generating copyout(x_(:),p_(:),v_(:))
         ...
```

```
root=1.0/sqrt(1.0+sum(p_**2))
!...
```

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```
!$acc parallel loop private(pp,root,qi,mi,wi) present(e,
↪  b) copy(list_of_particles)
```

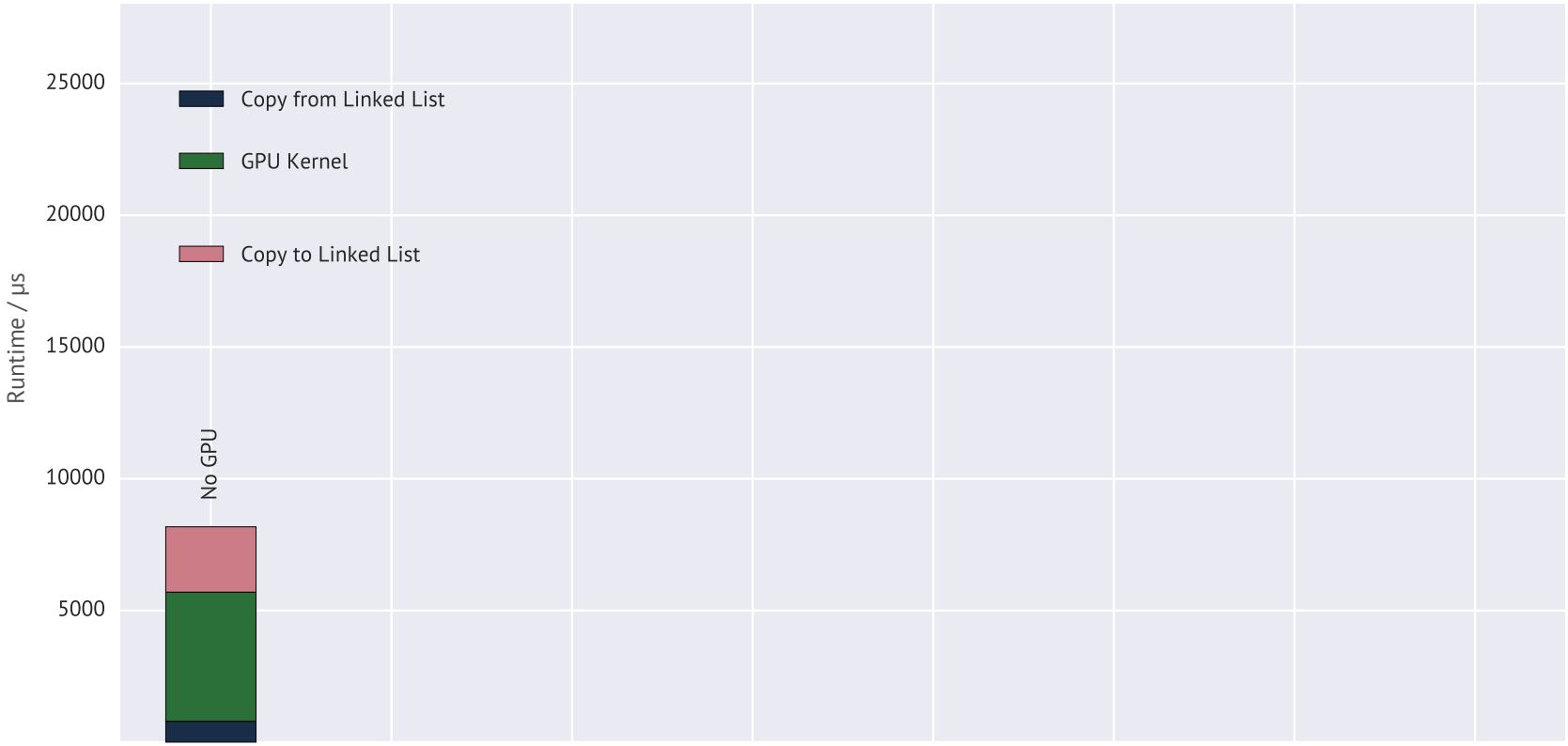
```
 End pusher:         92
 Start reducer
[zam449:24737] *** Process received signal ***
[zam449:24737] Signal: Segmentation fault (11)
[zam449:24737] Signal code: Address not mapped (1)
[zam449:24737] Failing at address: 0x693c239f98a0
[zam449:24737] *** End of error message ***
```

```
wi=p_prop(list_of_particles(i_particle)%id)%w

root=1.0/sqrt(1.0+sum(p_**2))
!...
```

Acceleration with OpenACC

Well…



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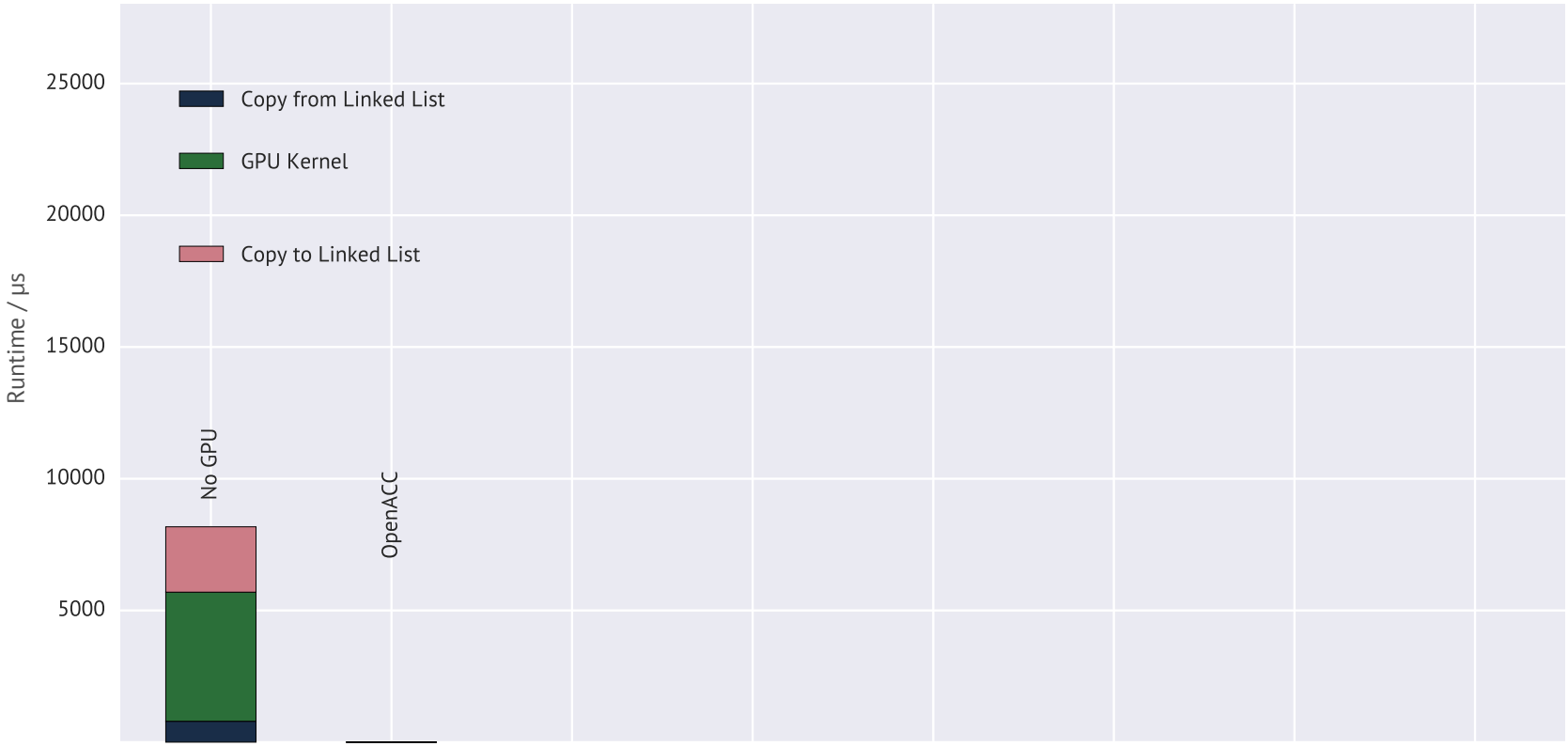

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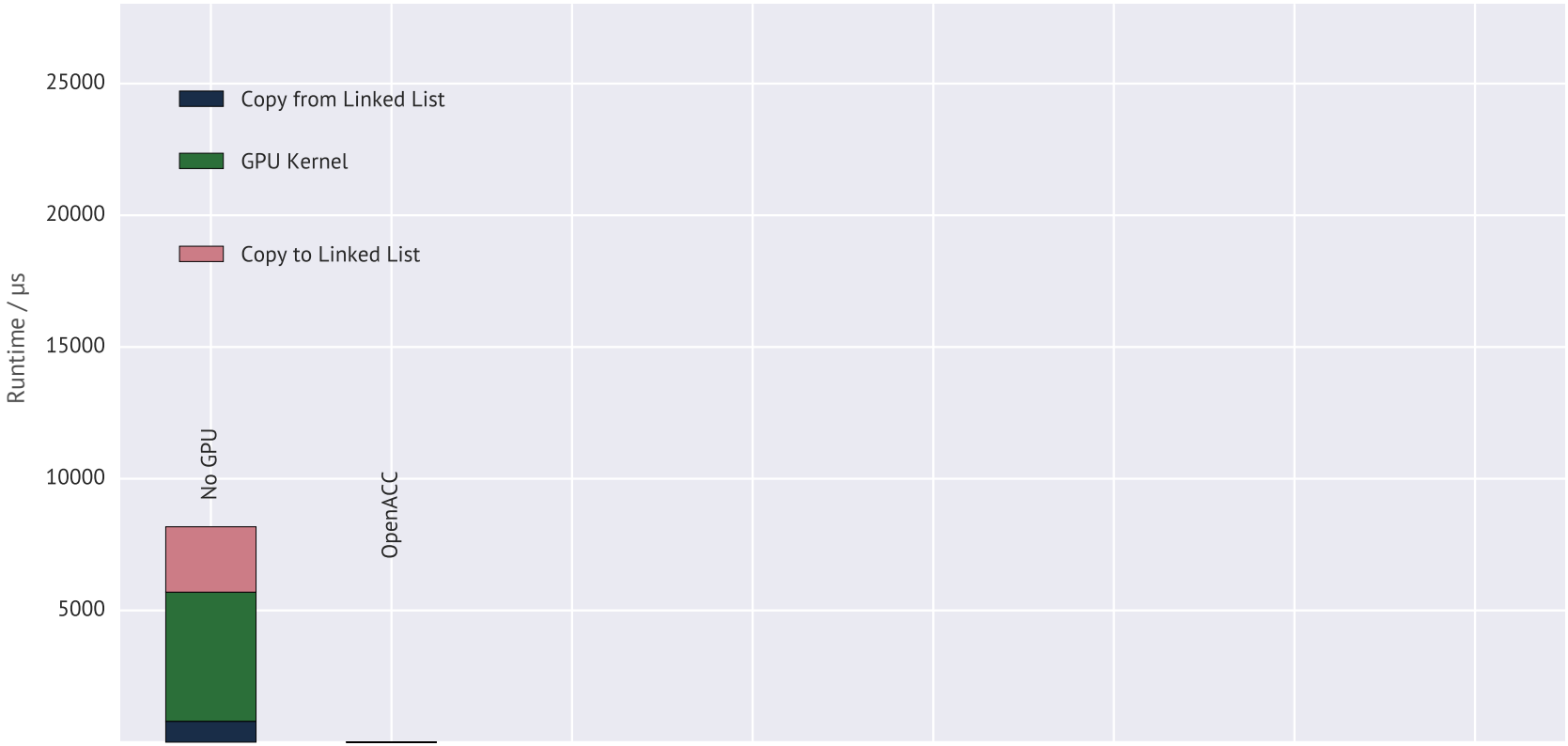

OpenACC?

At least a working version?!

- Changes for a *running* PGI OpenACC program

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- Changes for a *running* PGI OpenACC program
  - Unroll some operations on arrays

    PGI compiler silently/automatically generates temporary variables which it stumbles over during OpenACC translation step

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x_=list_of_particles(i_particle)%vec
p_=list_of_particles(i_particle)%pvec
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```

  - Explicitly stage private variables

```
!$acc loop private(bvp,x_,hh,jj,t,...
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  - Limit number of threads!

    Too much state?!

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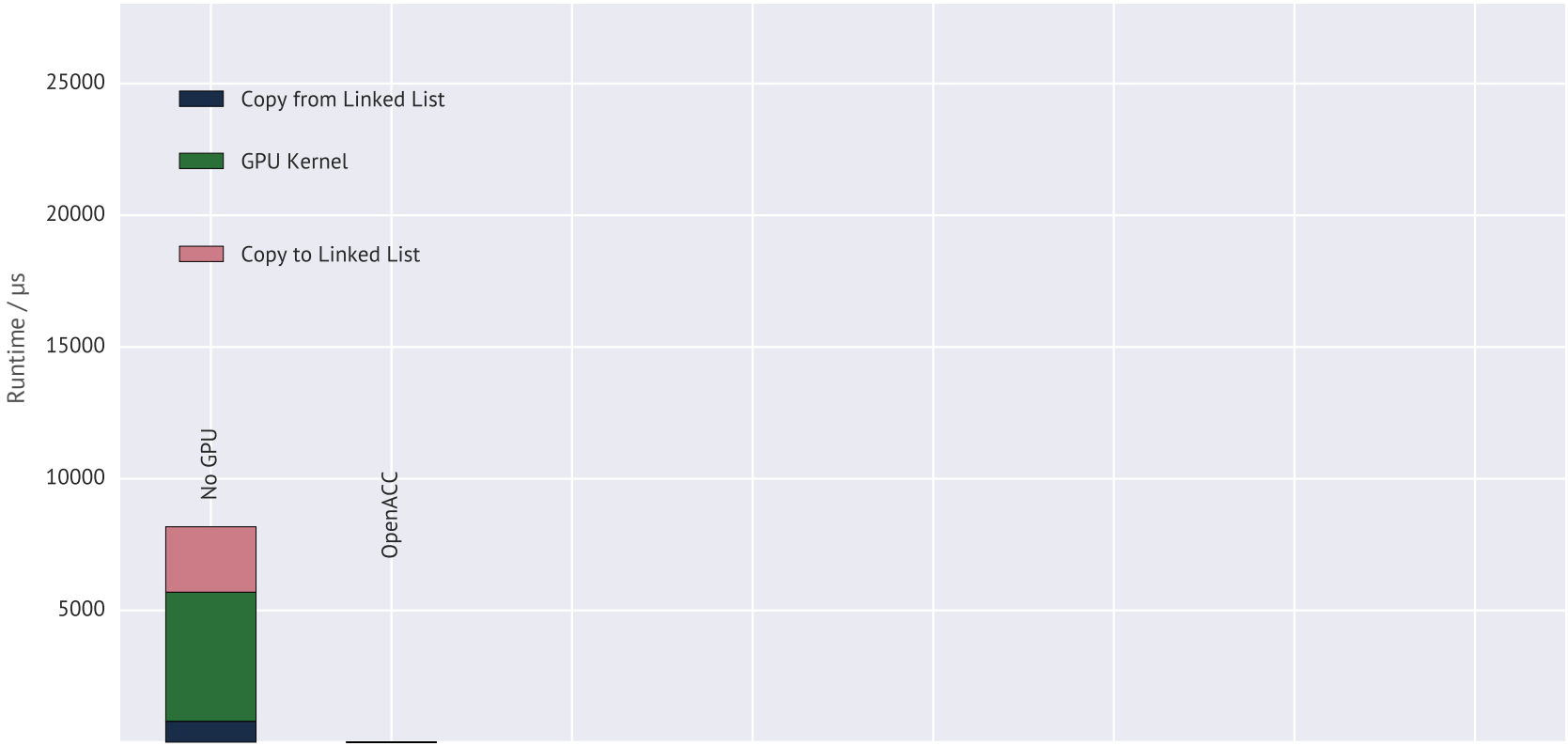
→ ***Slow!?***

OpenACC?

Slow?



OpenACC?

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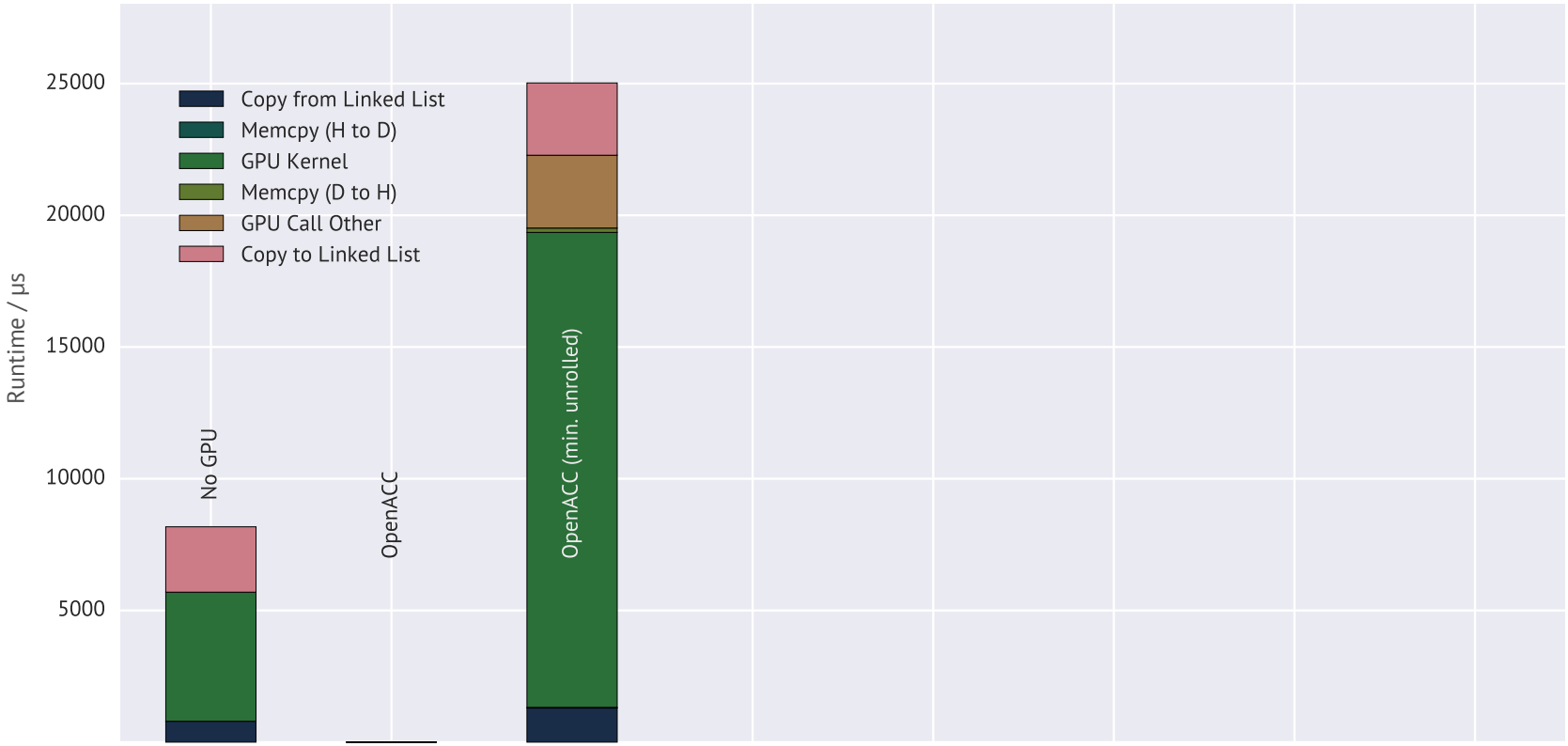

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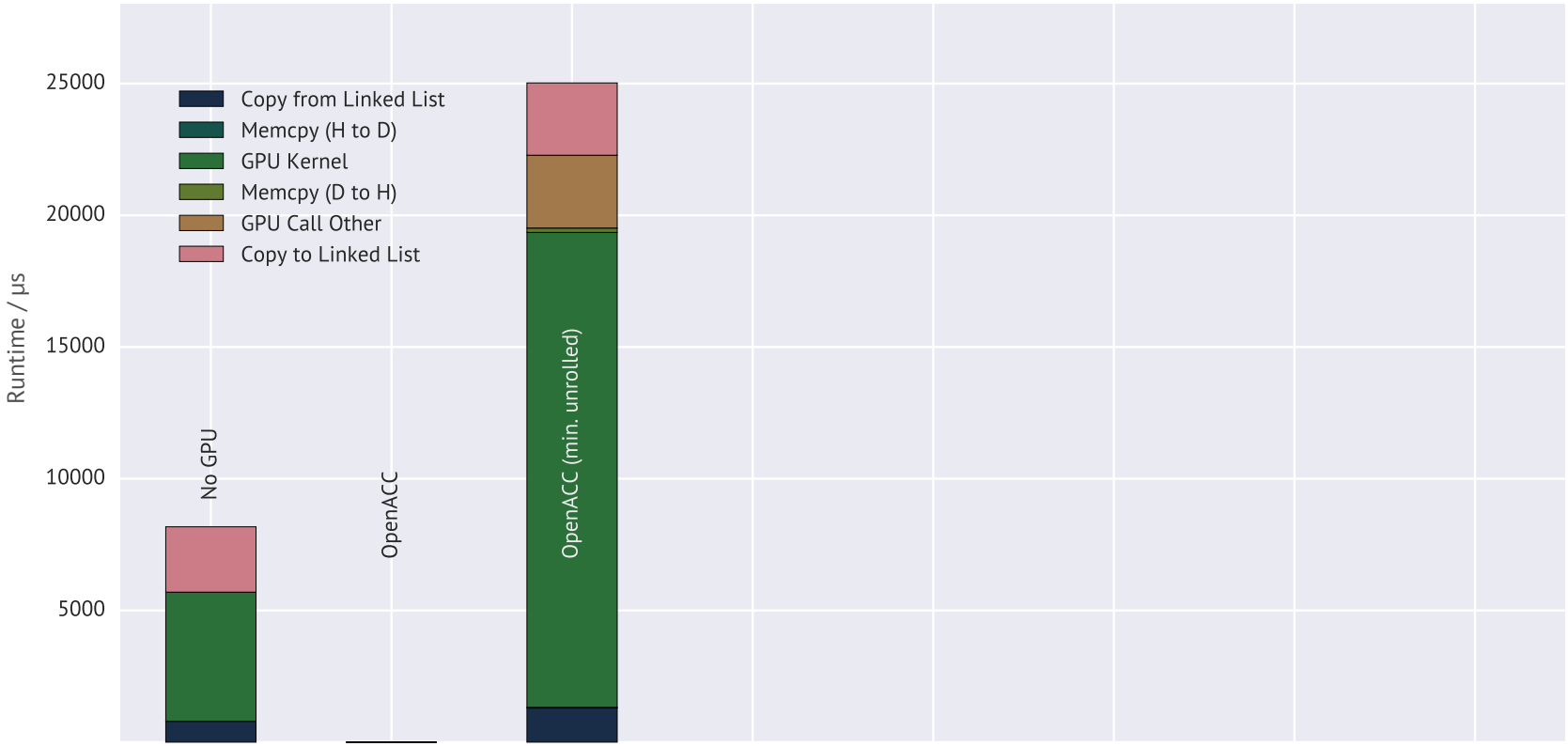

...?!

OpenACC with Speedup

Finally!

JÜLICH FORSCHUNGSZENTRUM

- Changes for a *fast* PGI OpenACC program

OpenACC with Speedup

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- Changes for a *fast* PGI OpenACC program
  - Replace all arrays with scalars, all operations on arrays with scalar operations

    Preprocessor macros to the rescue!

```
xi_1 = list_of_particles(i_particle)%vec(1)
xi_2 = list_of_particles(i_particle)%vec(2)
xi_3 = list_of_particles(i_particle)%vec(3)
pi_1 = list_of_particles(i_particle)%pvec(1)
! ...
```

OpenACC with Speedup

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push_particle_2d_2_3:
   875, include 'pic.in.gpu.fullyunrolled.F90'
      268, Generating present(e(:,:,:),b(:,:,:))
         Generating copy(list_of_particles(:))
         Accelerator kernel generated
         Generating Tesla code
        269, !$acc loop gang, vector(128) ! blockidx%x threadidx%x
      268, Generating copyin(p_prop(list_of_particles%id))
```

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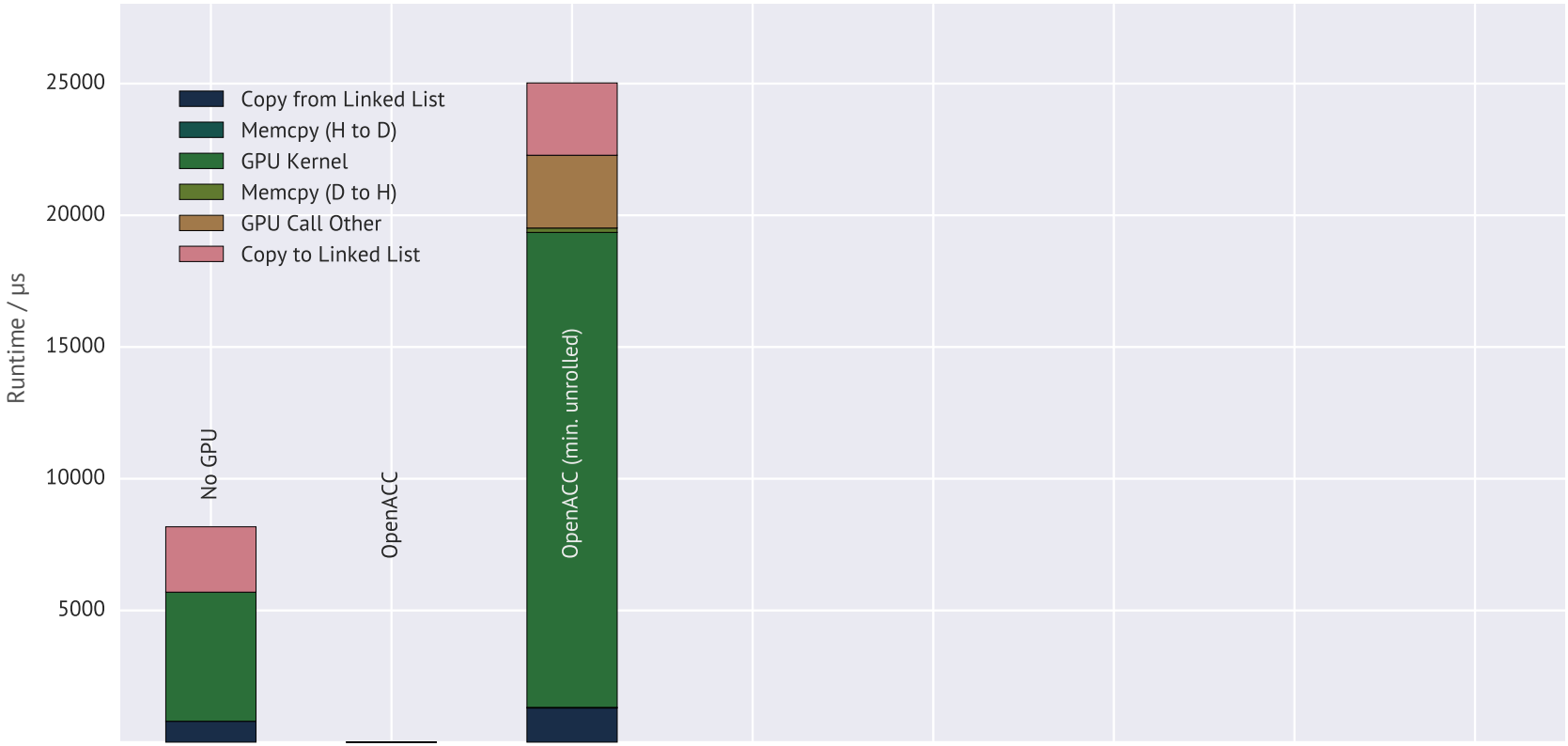
OpenACC!

It's faster?



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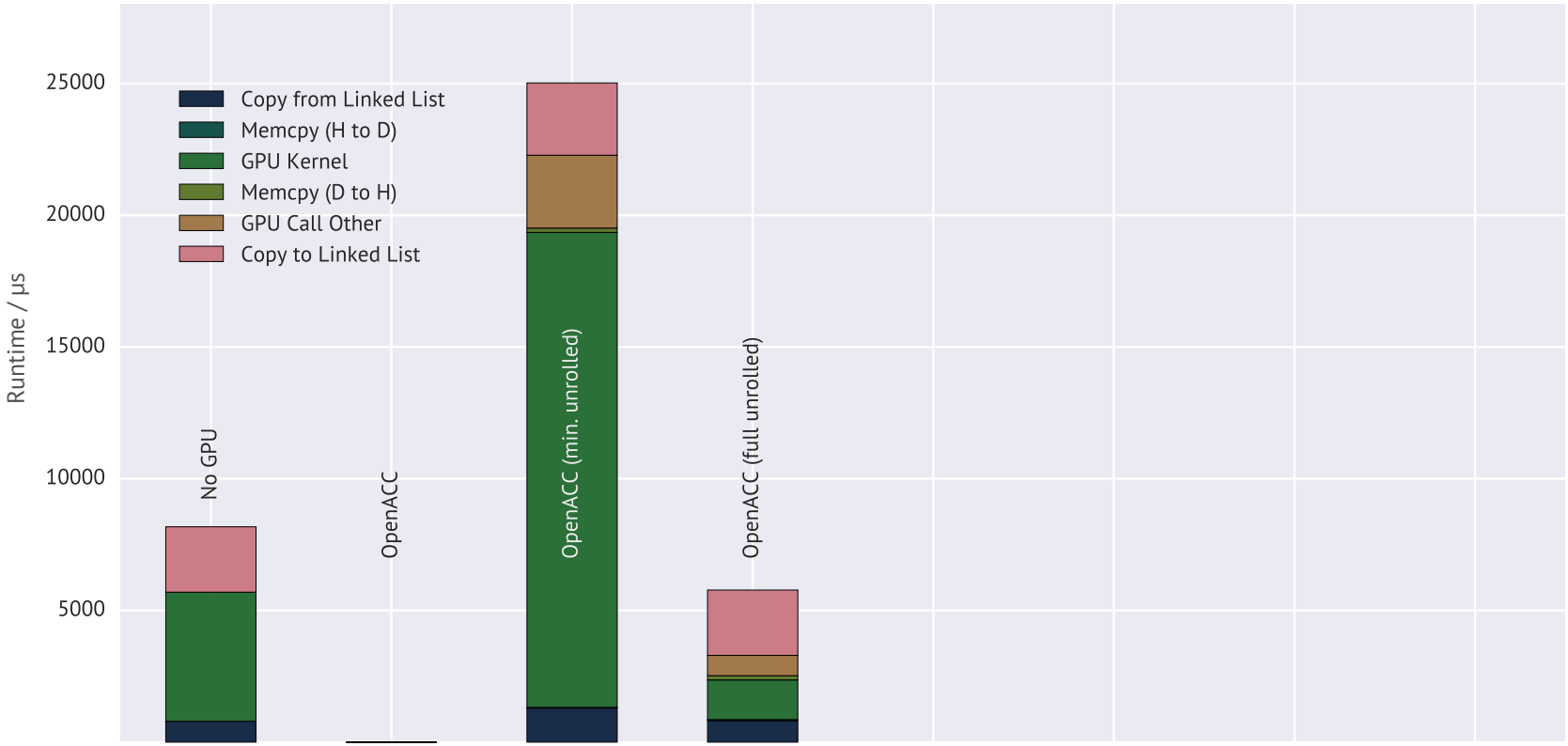

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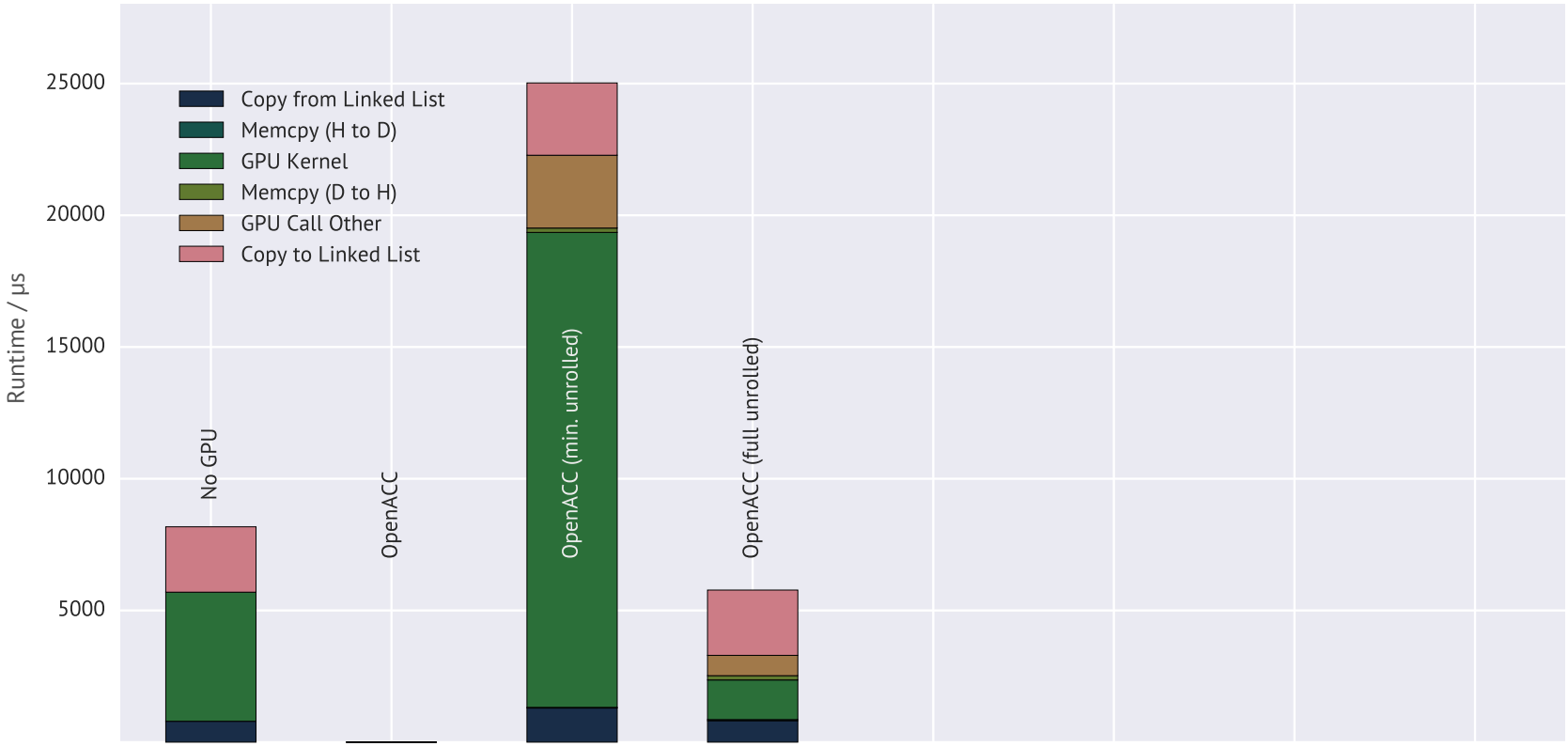

CUDA Fortran

Let's bring out the big guns

JÜLICH FORSCHUNGSZENTRUM

- At this point, code closer to rewritten C code than to original code
- Not very OpenACC-ish

CUDA Fortran

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- Different approach: **CUDA Fortran**!

CUDA Fortran

Let's bring out the big guns

JÜLICH FORSCHUNGSZENTRUM

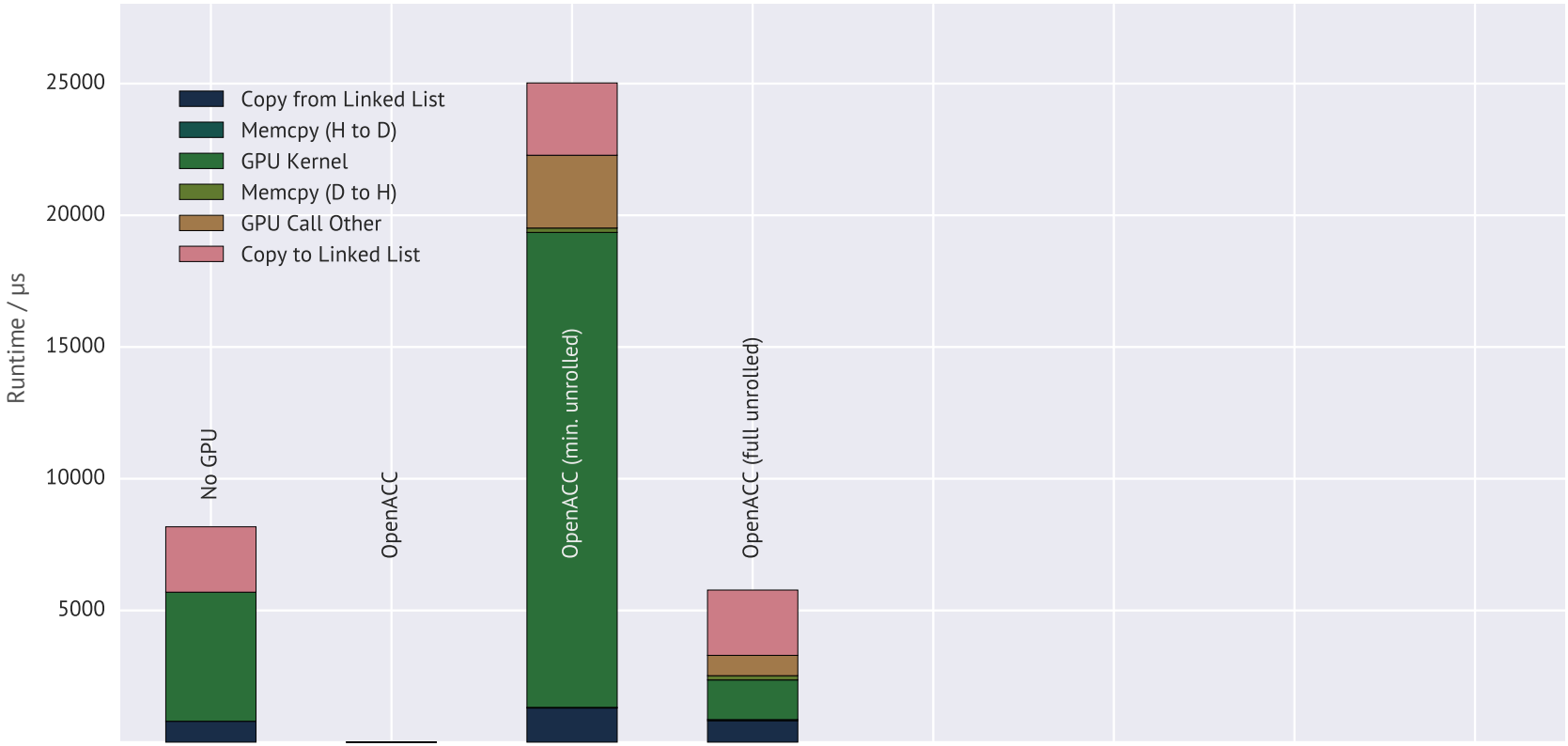
- At this point, code closer to rewritten C code than to original code
- Not very OpenACC-ish
- Different approach: **CUDA Fortran**!
- Can also be *portable* with pre-processor guards

```
#ifdef _CUDA
  i = blockDim%x * (blockIdx%x - 1) + threadIdx%x
#else
  do i = lbound(a, 1), ubound(a, 1)
#endif
```

- Original code can be kept!

CUDA Fortran!

A good time?



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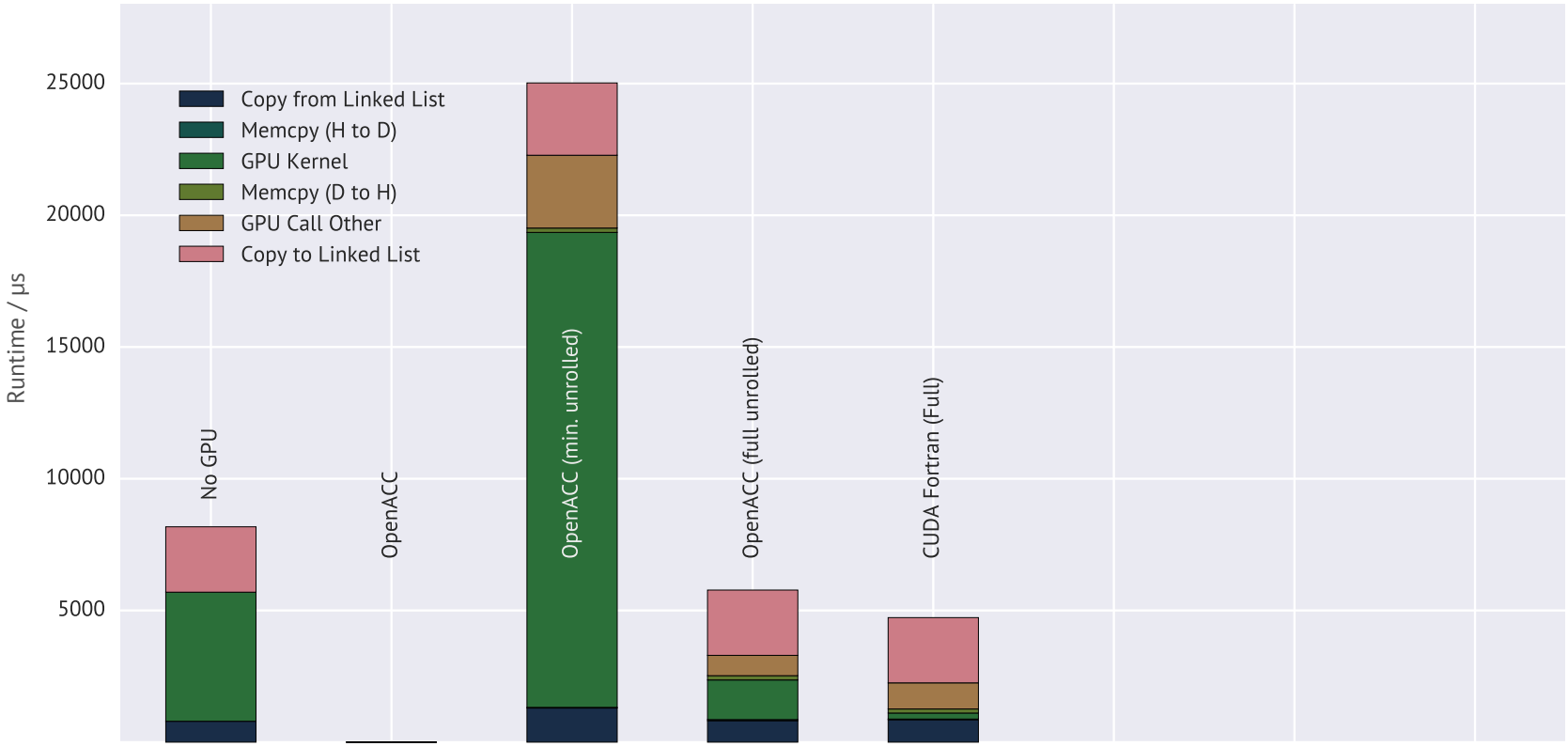

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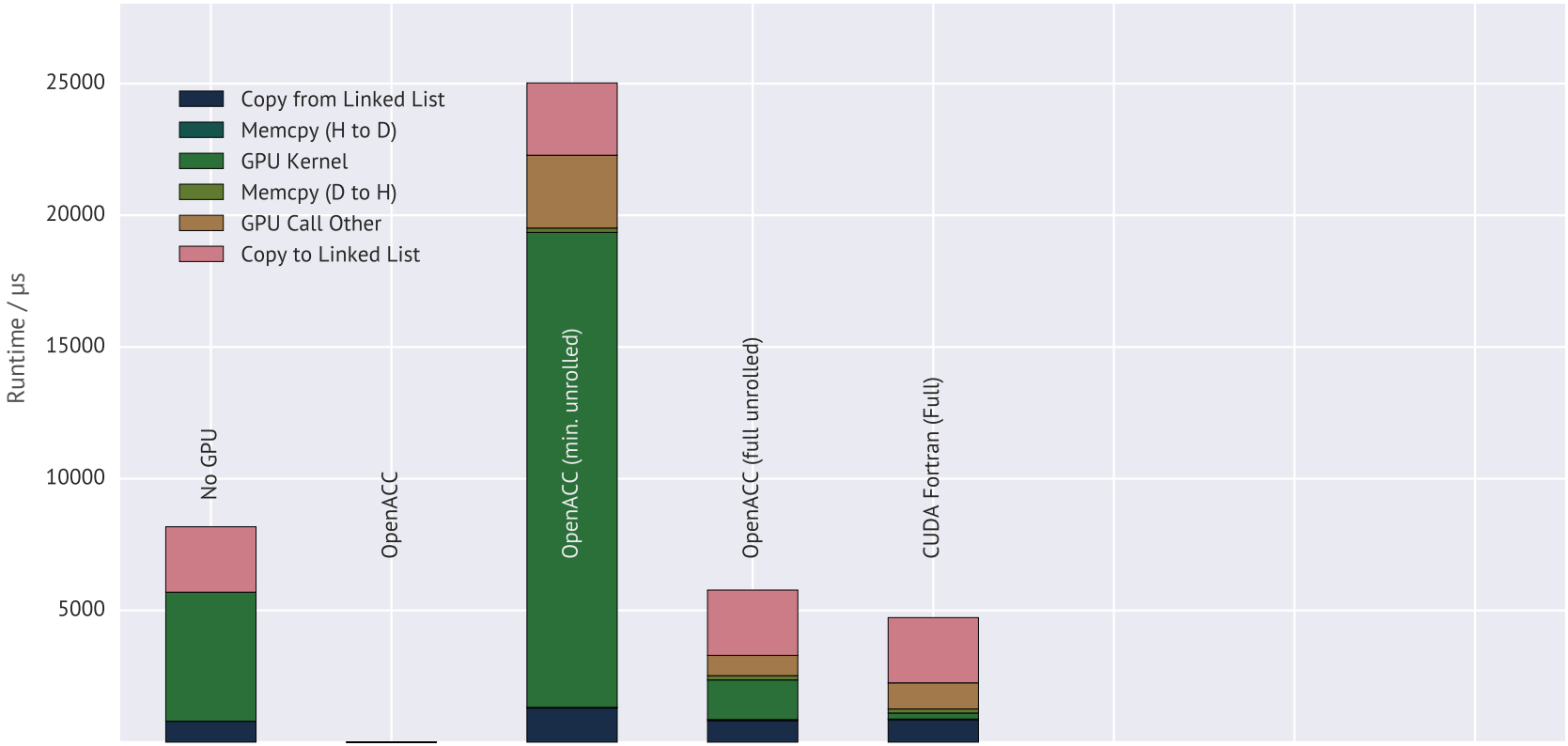

Hybrid CUDA OpenACC

Mingling

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- Already in last version:

  OpenACC Maxwell Solver, *helper* data (scalars, 3D vectors, fields)

  CUDA Particle Pusher, particle momenta / positions

Hybrid CUDA OpenACC

Mingling

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- Already in last version:

  OpenACC Maxwell Solver, *helper* data (scalars, 3D vectors, fields)

  CUDA Particle Pusher, particle momenta / positions

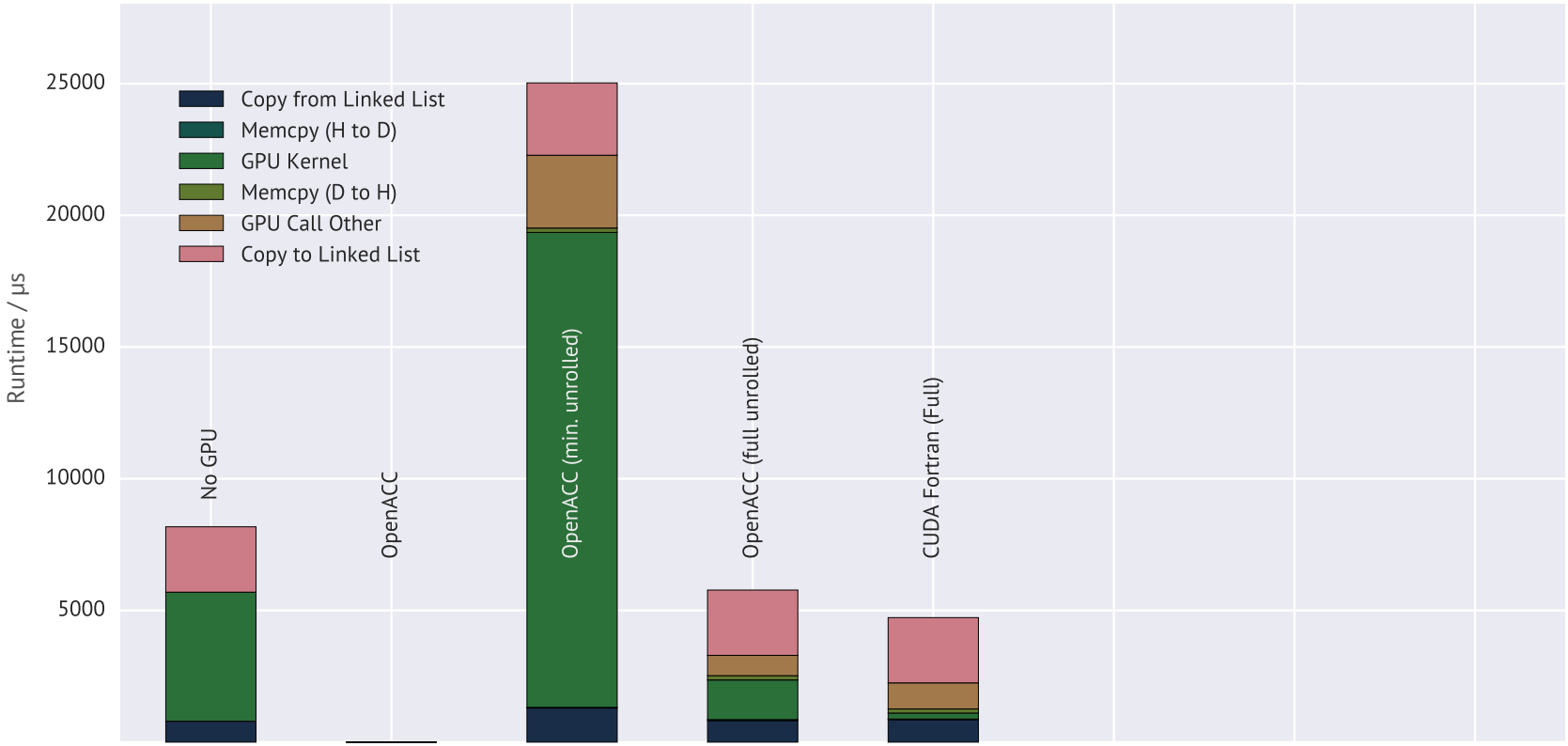
→ Evaluation of

  — Full data handling with OpenACC

  — Full data handling with OpenACC, pinned host memory

OpenACC data handling

OpenACC copy is reasonable



OpenACC data handling

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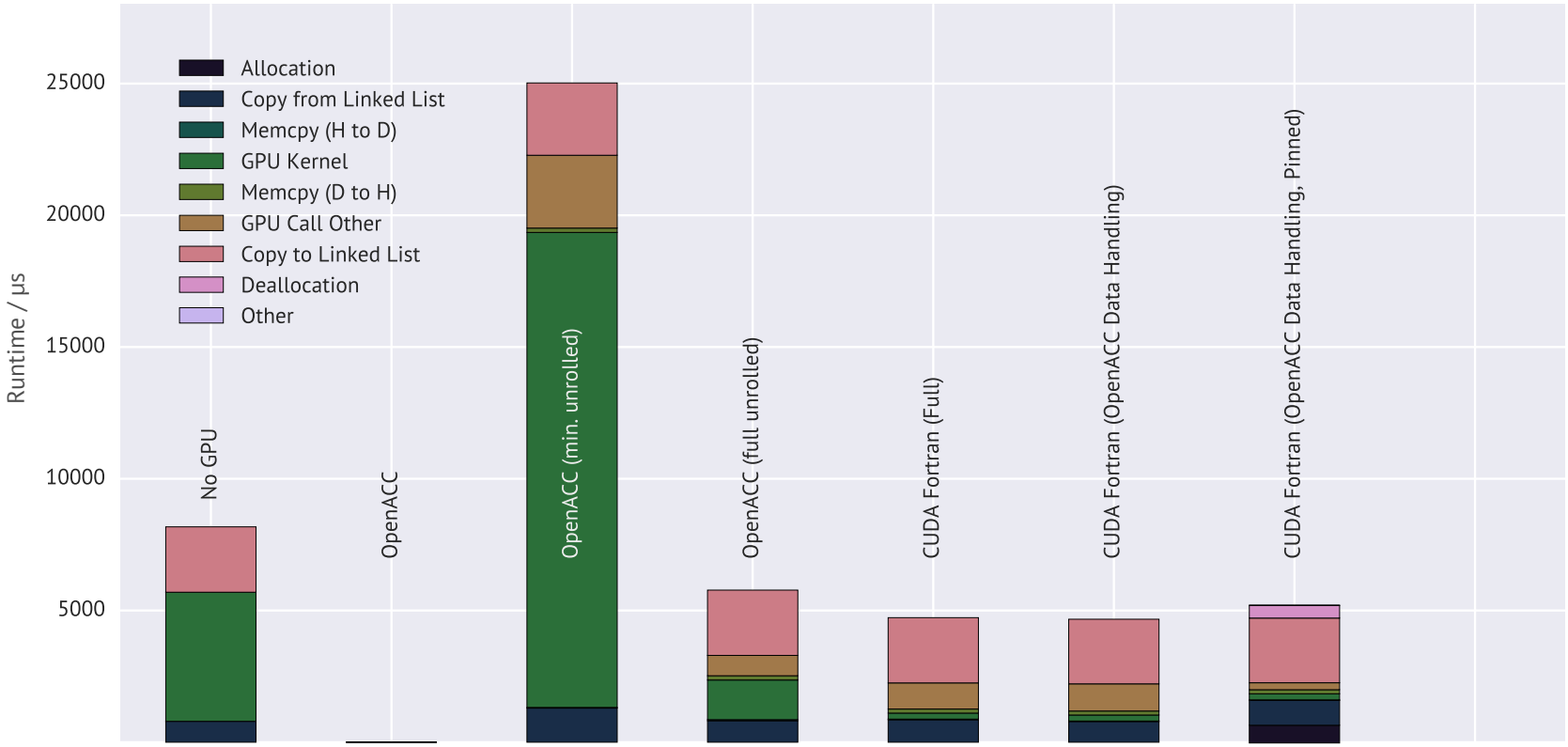
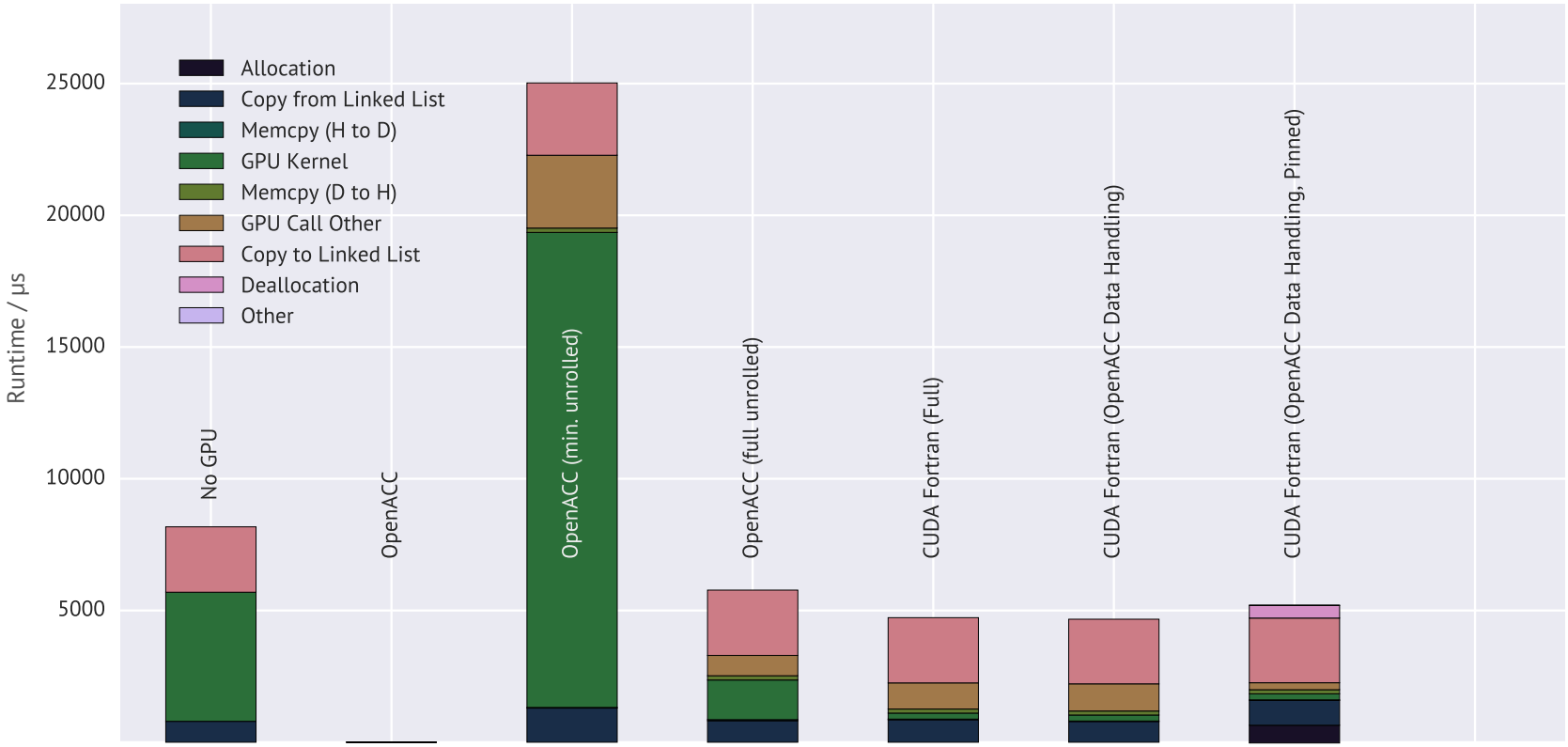


OpenACC data handling

OpenACC copy is reasonable



Data Structure of Particles

AoS → SoA

- Original data structure: Array of structs (AoS)

```
type particle
   sequence
   real(dp_kind) :: vec(3), pvec(3)
end type particle
type(particle), dimension(:), allocatable ::
↪  list_of_particles
```

Data Structure of Particles

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```
type particle
   sequence
   real(dp_kind) :: vec(3), pvec(3)
end type particle
type(particle), dimension(:), allocatable ::
↪  list_of_particles
```

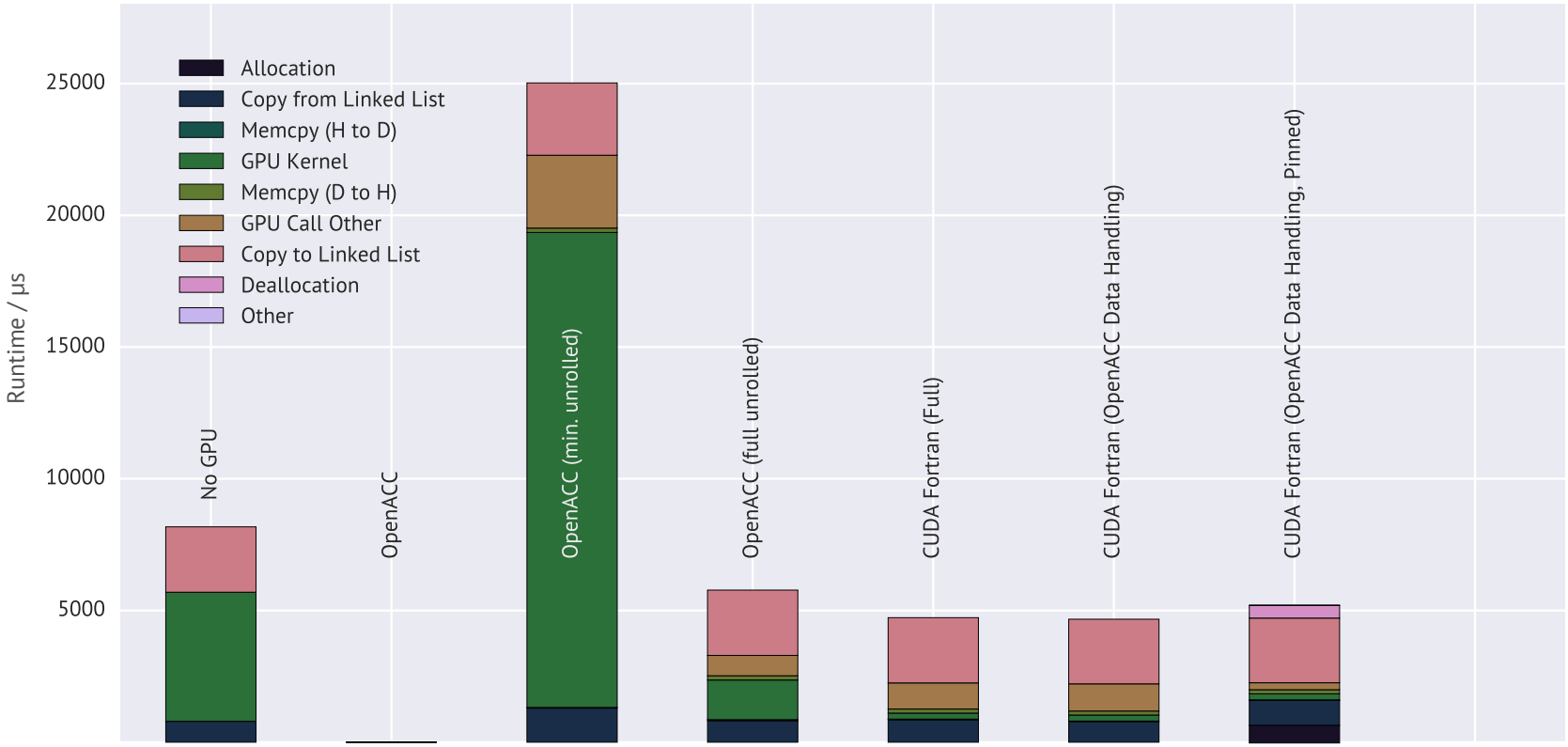
- Align data for coalesced GPU access (SoA)

```
type posmom
  real(dp_kind), dimension(:), allocatable :: x, y, z, px,
  ↪  py, pz
end type posmom
type(posmom) :: soa_list_of_particles
```

- Data only re-allocated when size changes

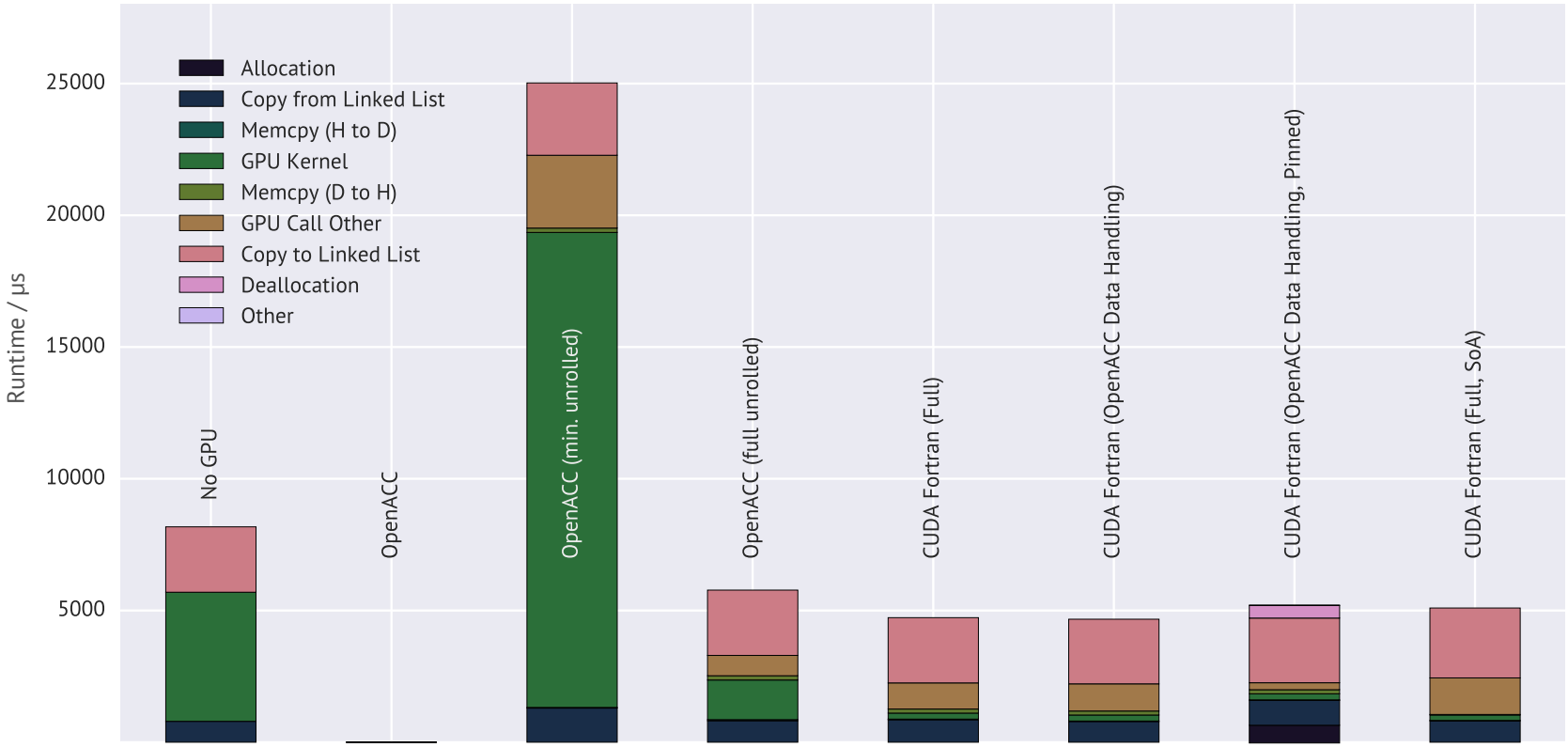
SoA Data Layout

Worth only if data is touched anyway



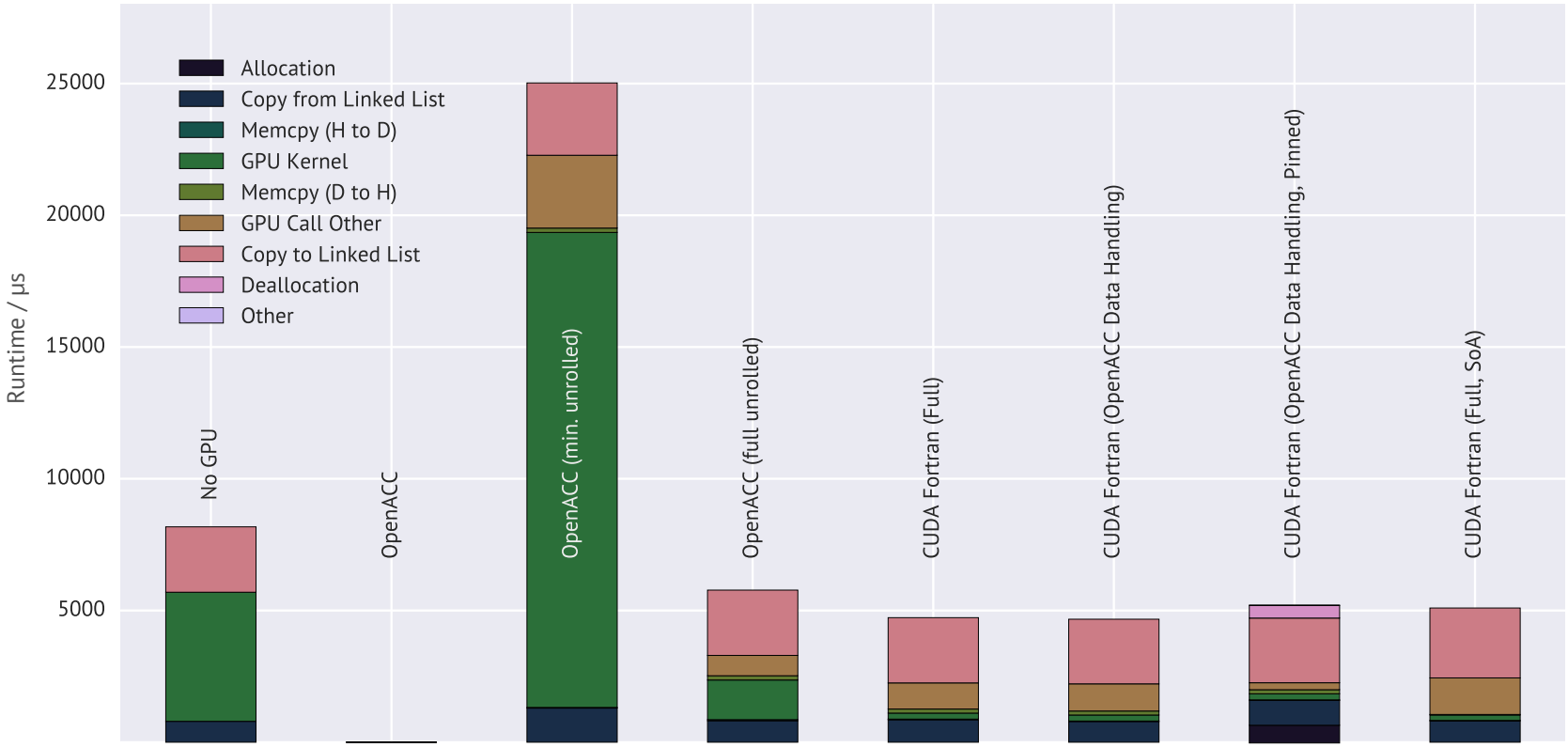
SoA Data Layout

Worth only if data is touched anyway



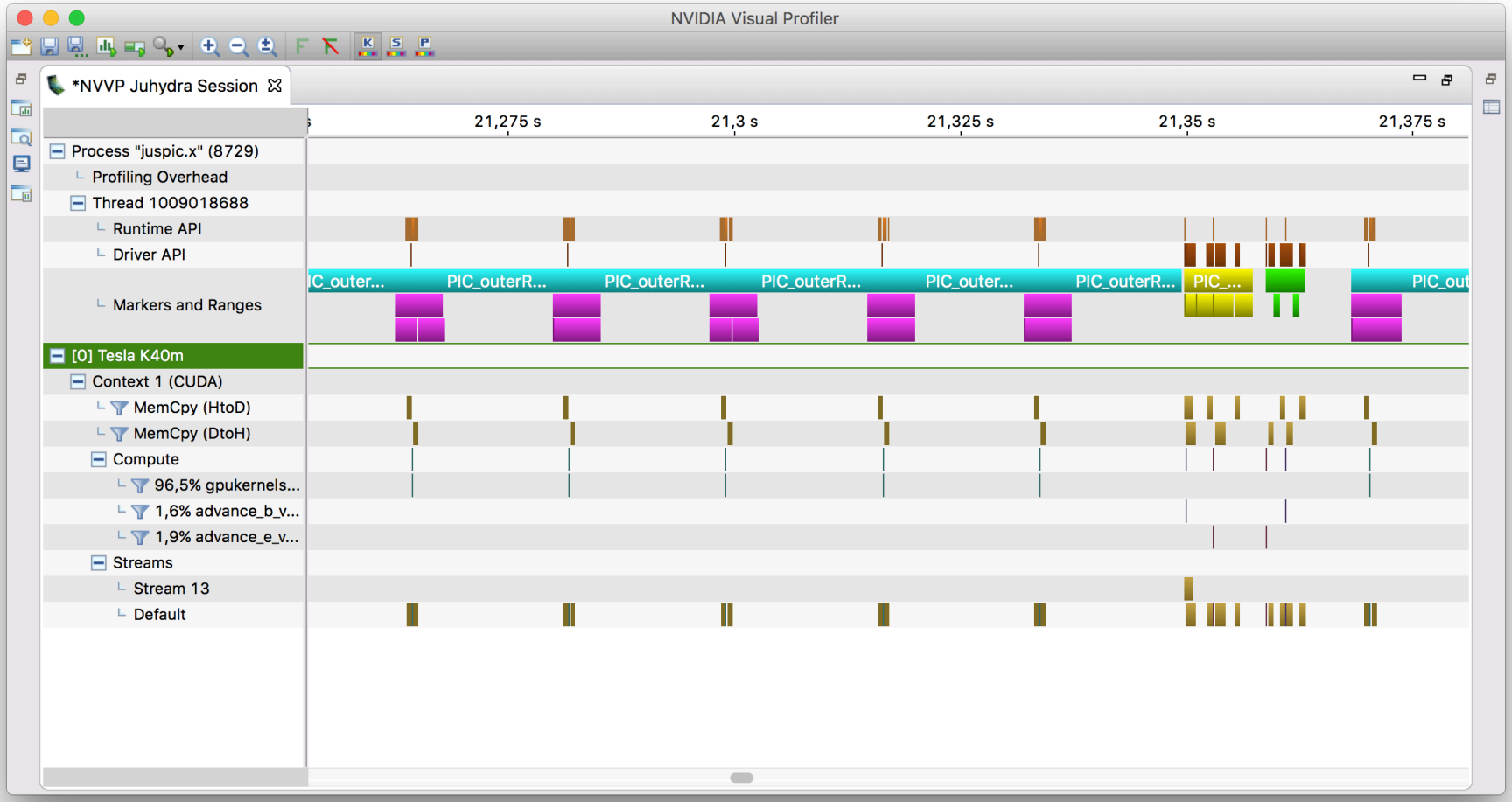
SoA Data Layout

Worth only if data is touched anyway

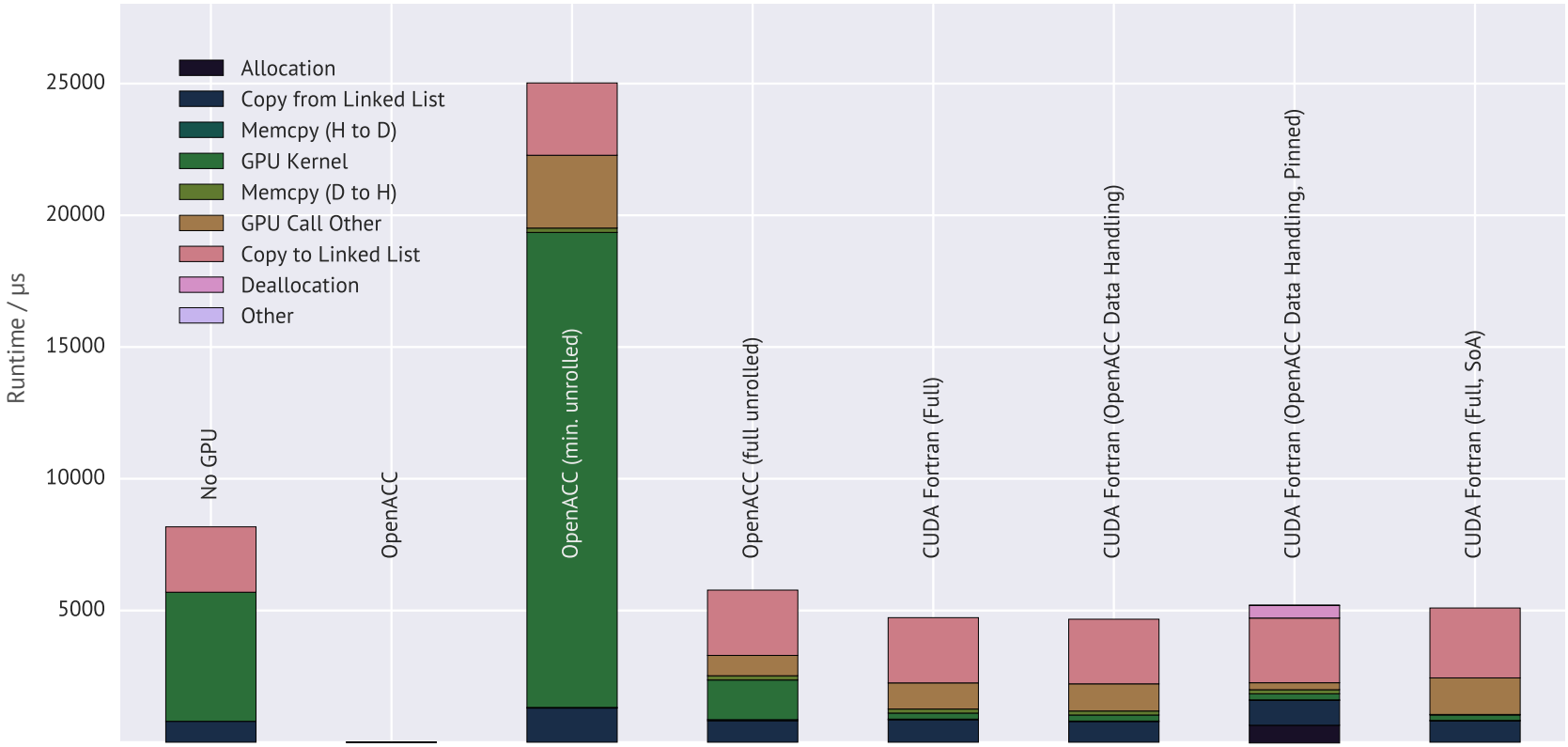


Visual Profiler

CUDA Fortran (Full, SoA)

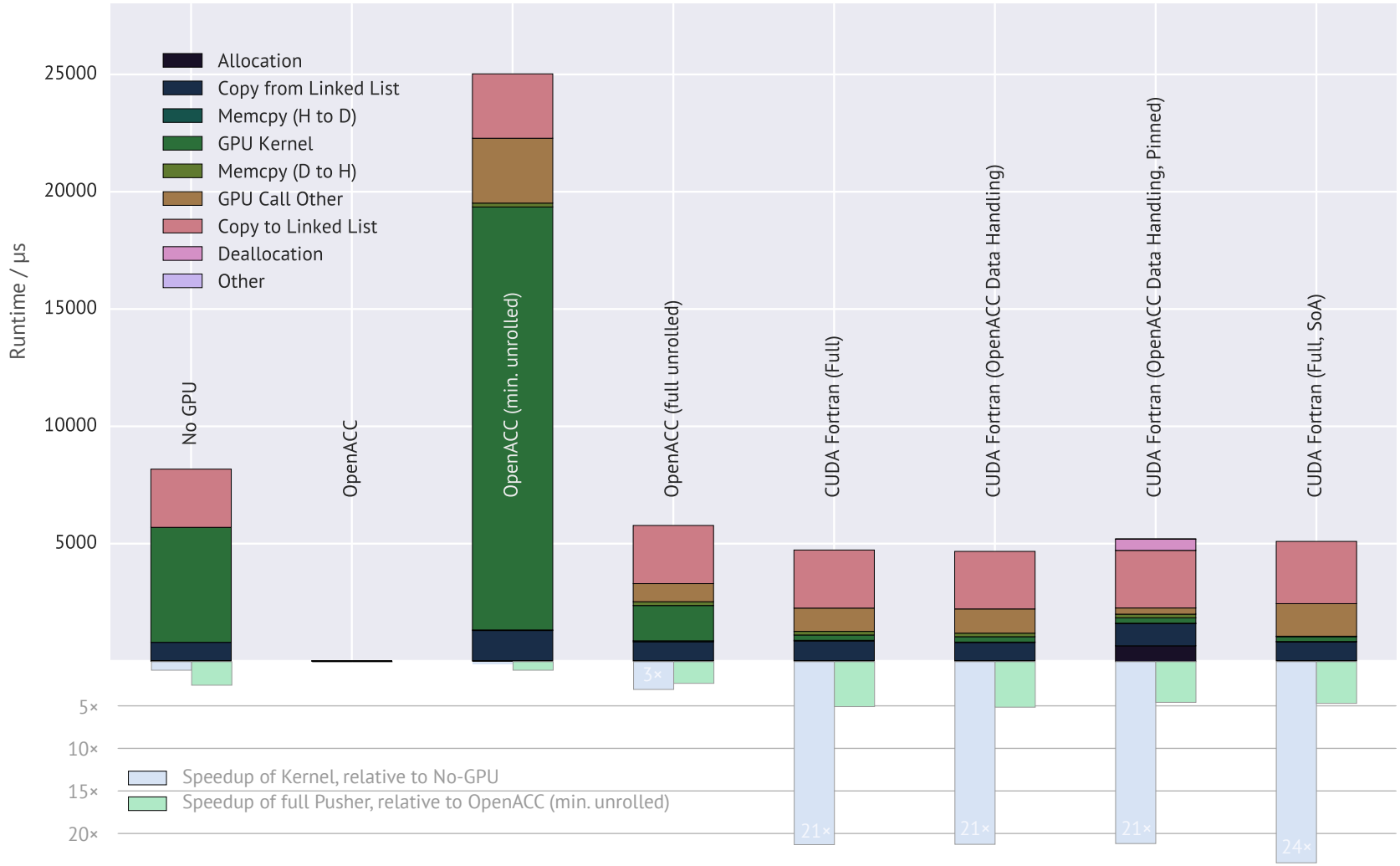


Speed-Up


Allocation
Copy from Linked List
Memcpy (H to D)
GPU Kernel
Memcpy (D to H)
GPU Call Other
Copy to Linked List
Deallocation
Other
Runtime / µs
25000
20000
15000
10000
5000
No GPU
OpenACC
OpenACC (min. unrolled)
OpenACC (full unrolled)
CUDA Fortran (Full)
CUDA Fortran (OpenACC Data Handling)
CUDA Fortran (OpenACC Data Handling, Pinned)
CUDA Fortran (Full, SoA)

Speed-Up

Kernel to CPU; Full pusher to OpenACC



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Performance Model

Introduction

Some information

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- Simple **information exchange model**

$$t(N_{\text{part}}) = \alpha + I(N_{\text{part}})/\beta$$

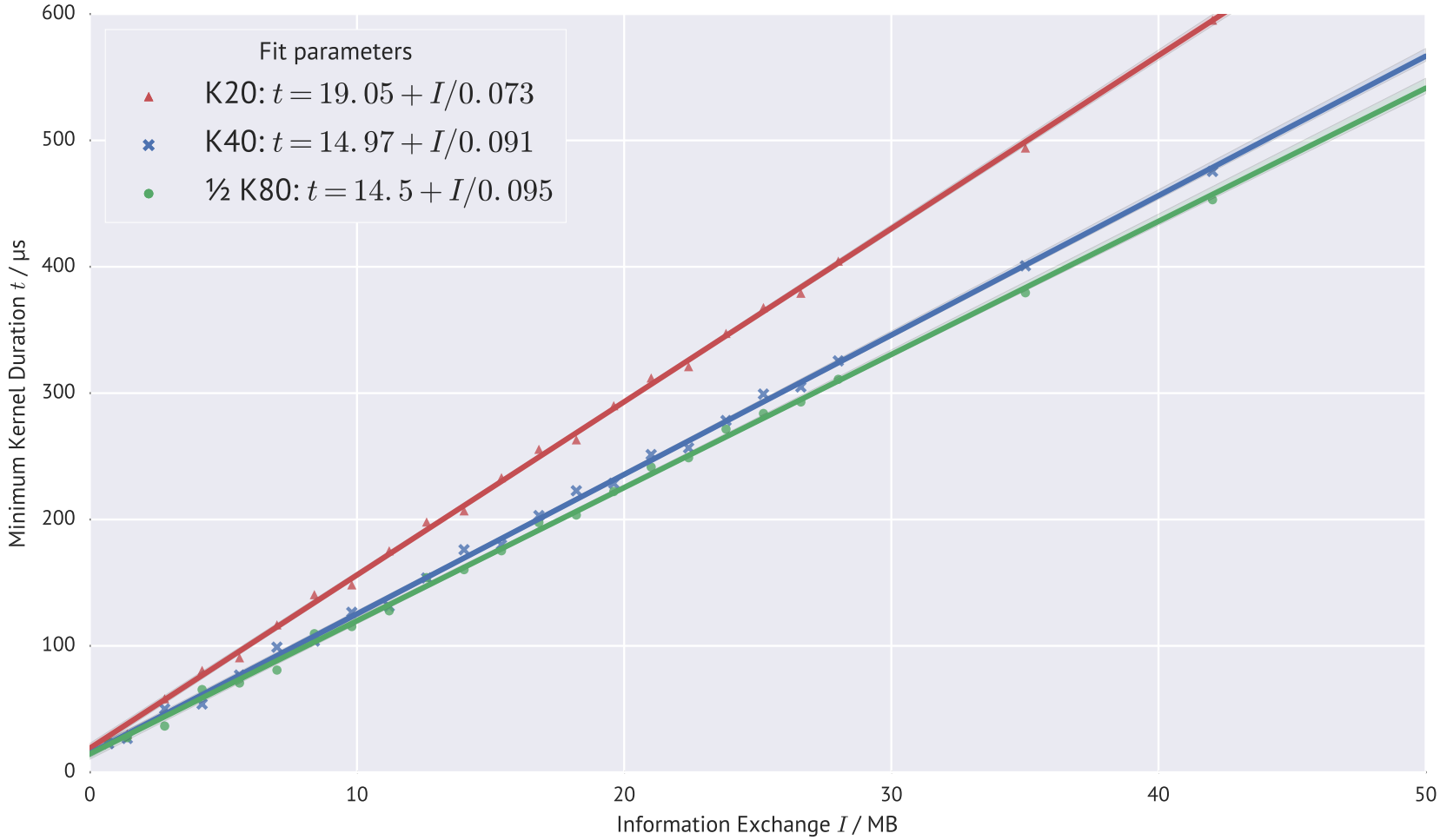
N_{part}	Number of particles processed
t	Duration of execution (in s)
I	Amount of information exchanged (in B)
α	Offset (*zero-data latency*); fit parameter
β	Slope (*effective bandwidth*); fit parameter

- Hypothesis: JuSPIC's GPU performance is largely limited by available bandwidth

$\rightarrow$ β is lower limit of exploited bandwidth

Bandwidth Determination

GPU clock fixed to maximum value



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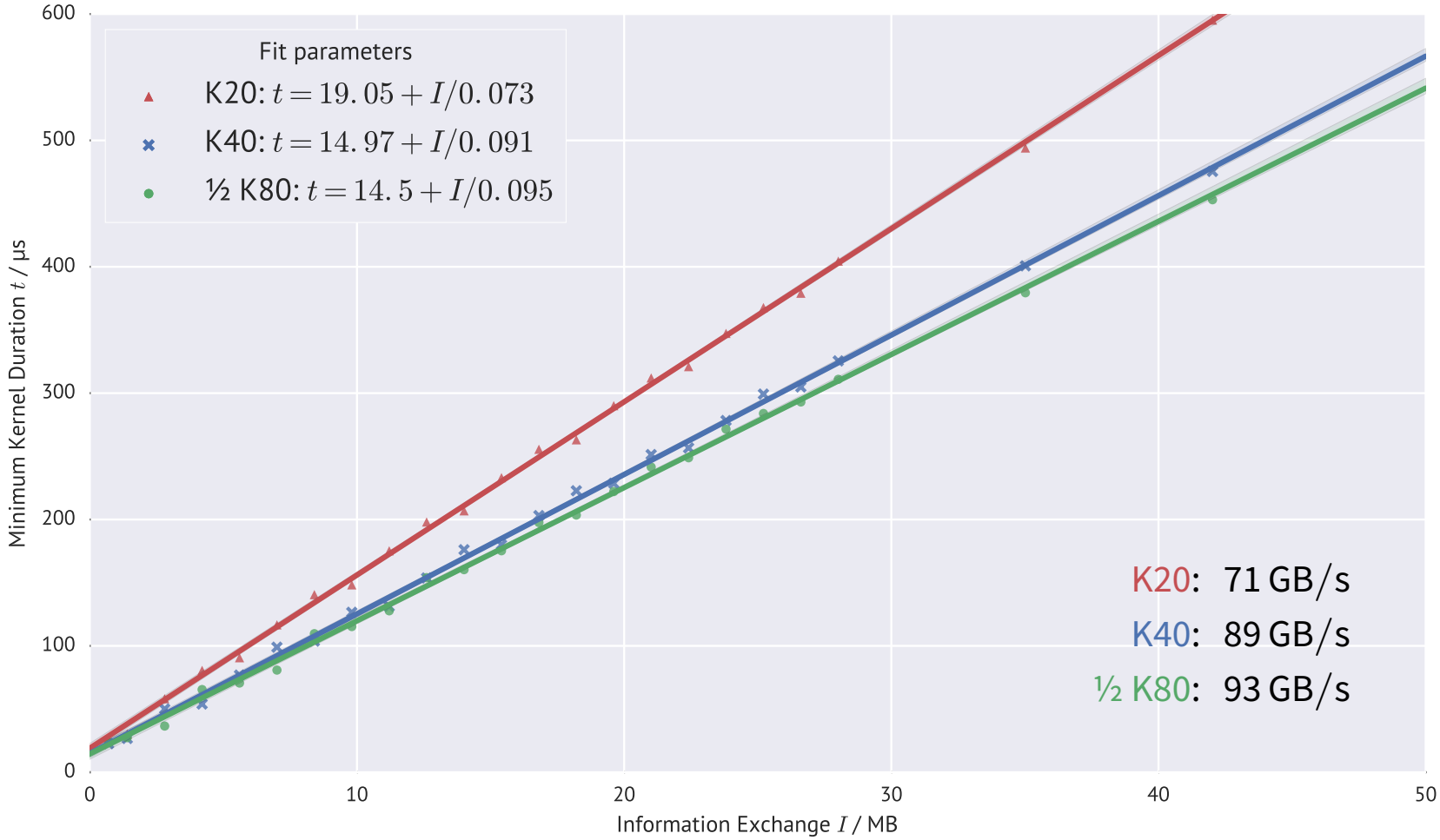

Bandwidth Determination

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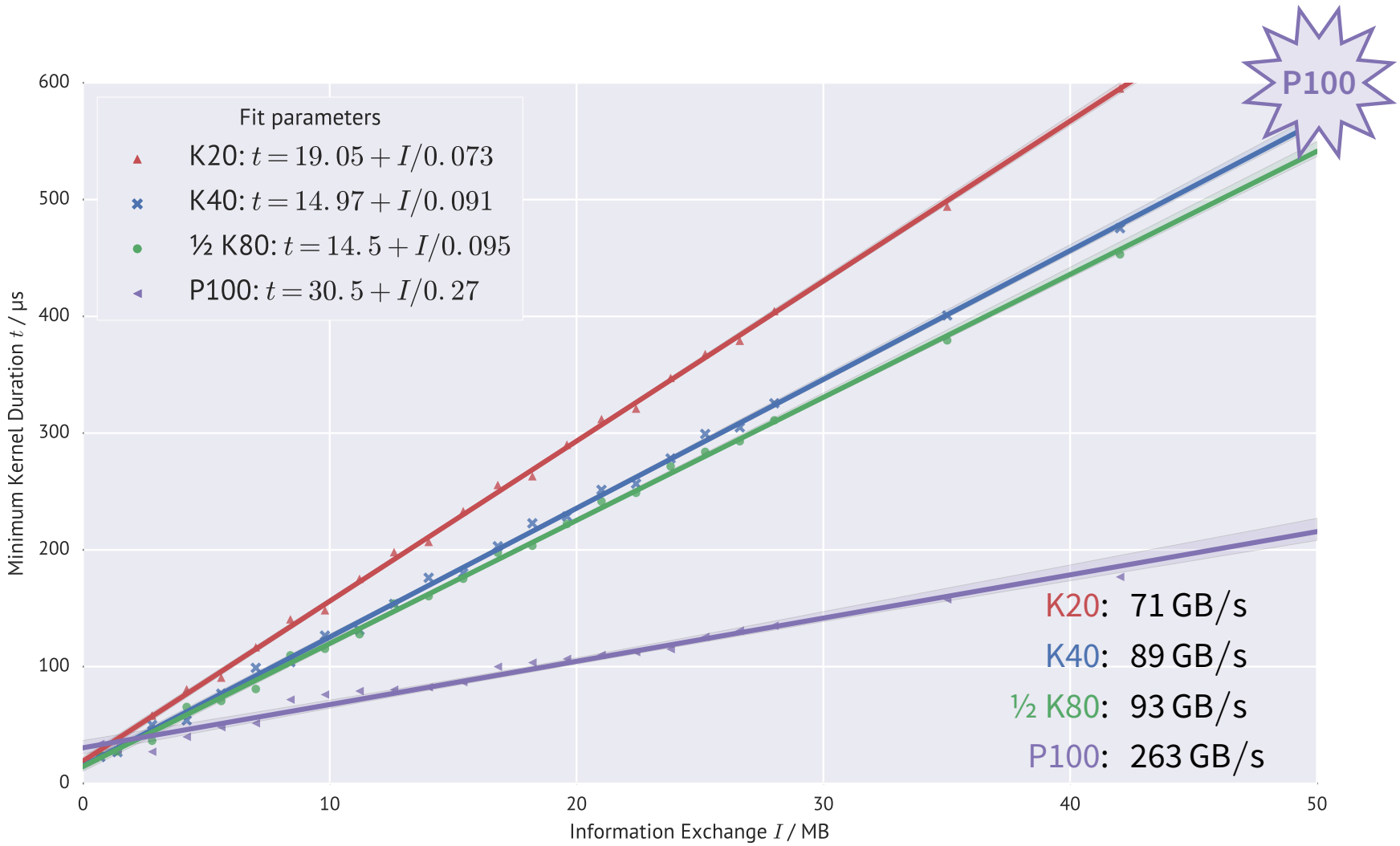
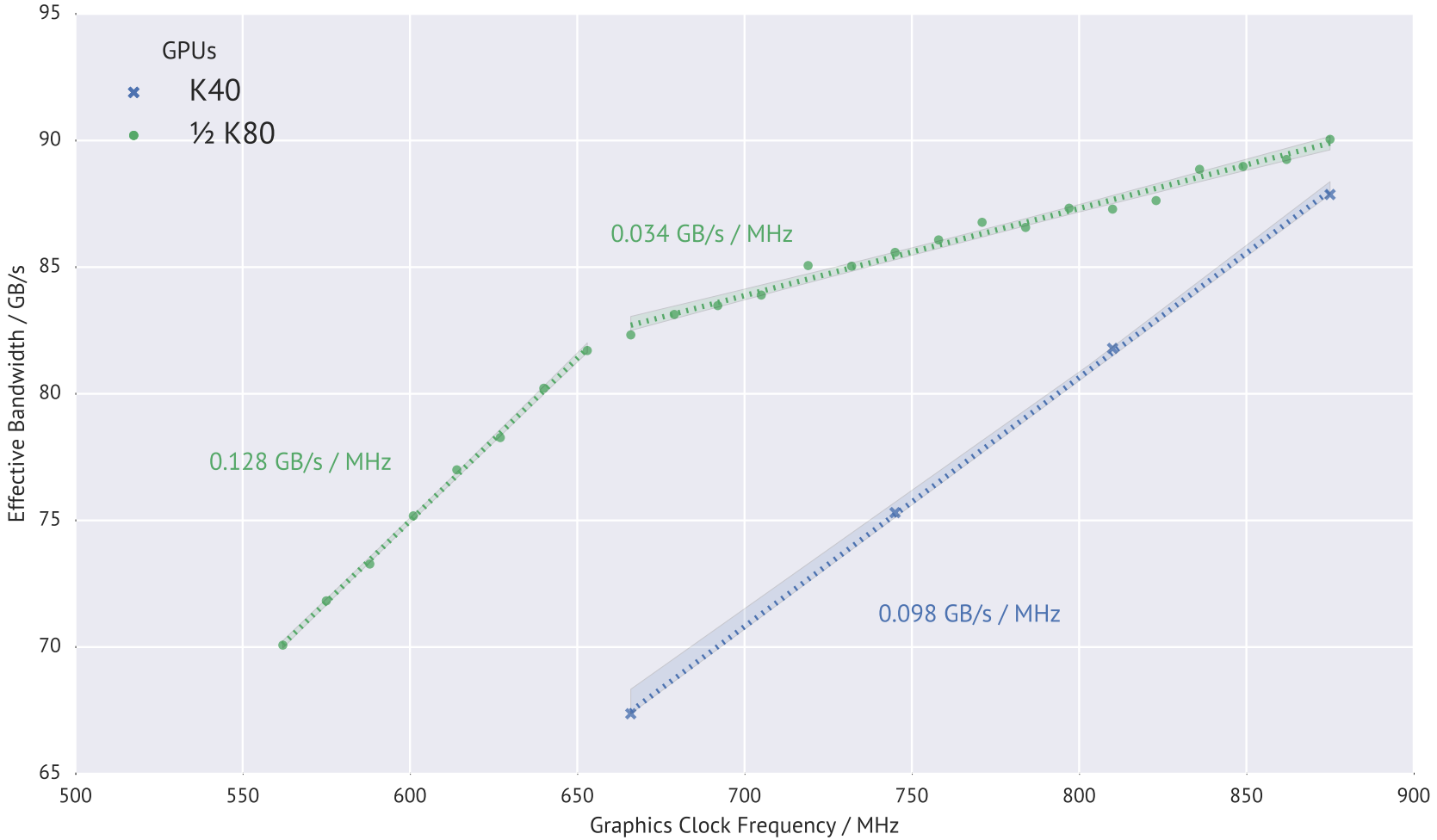


Bandwidth vs. Clock Frequency

Graphics clock frequency



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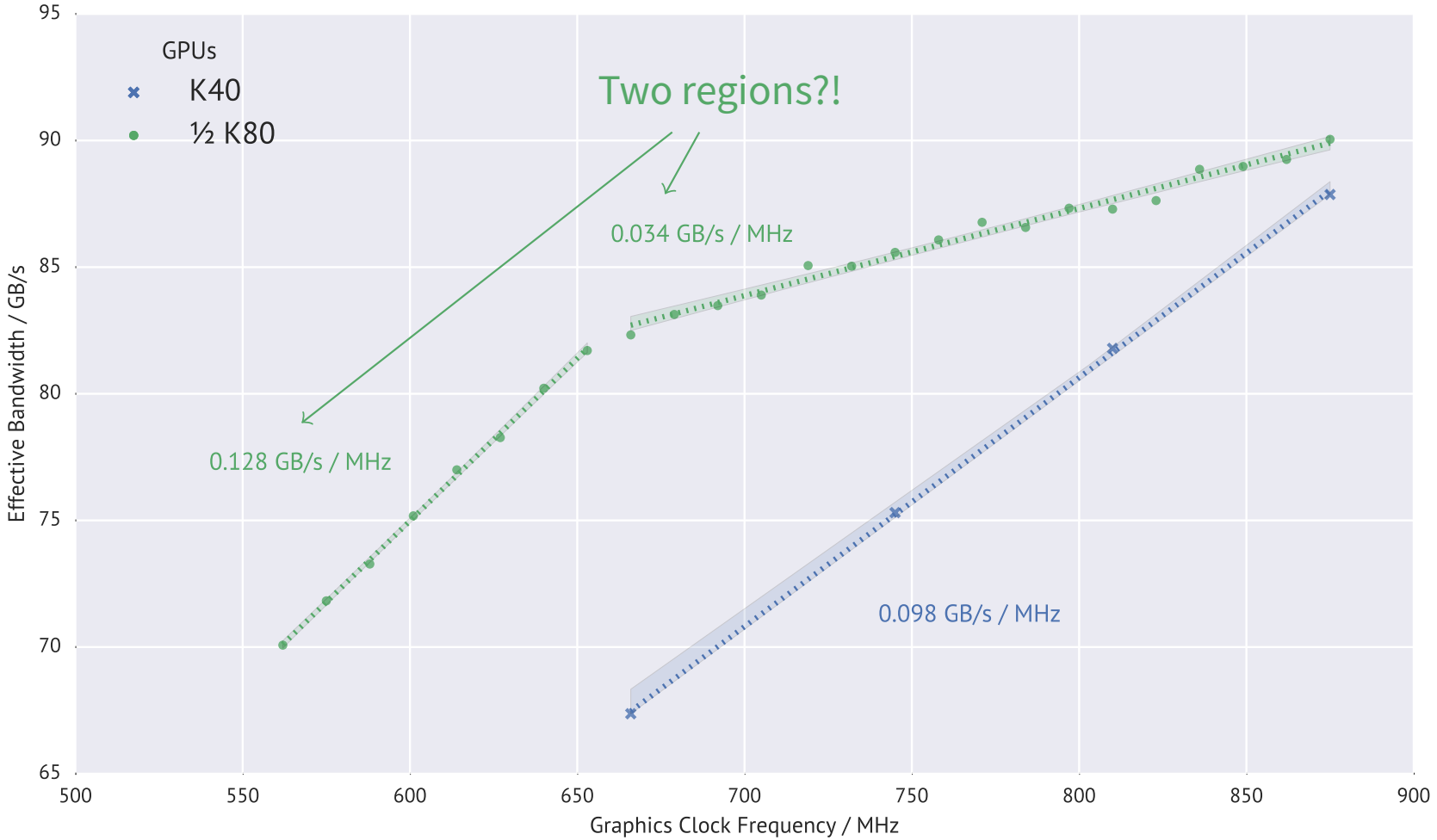
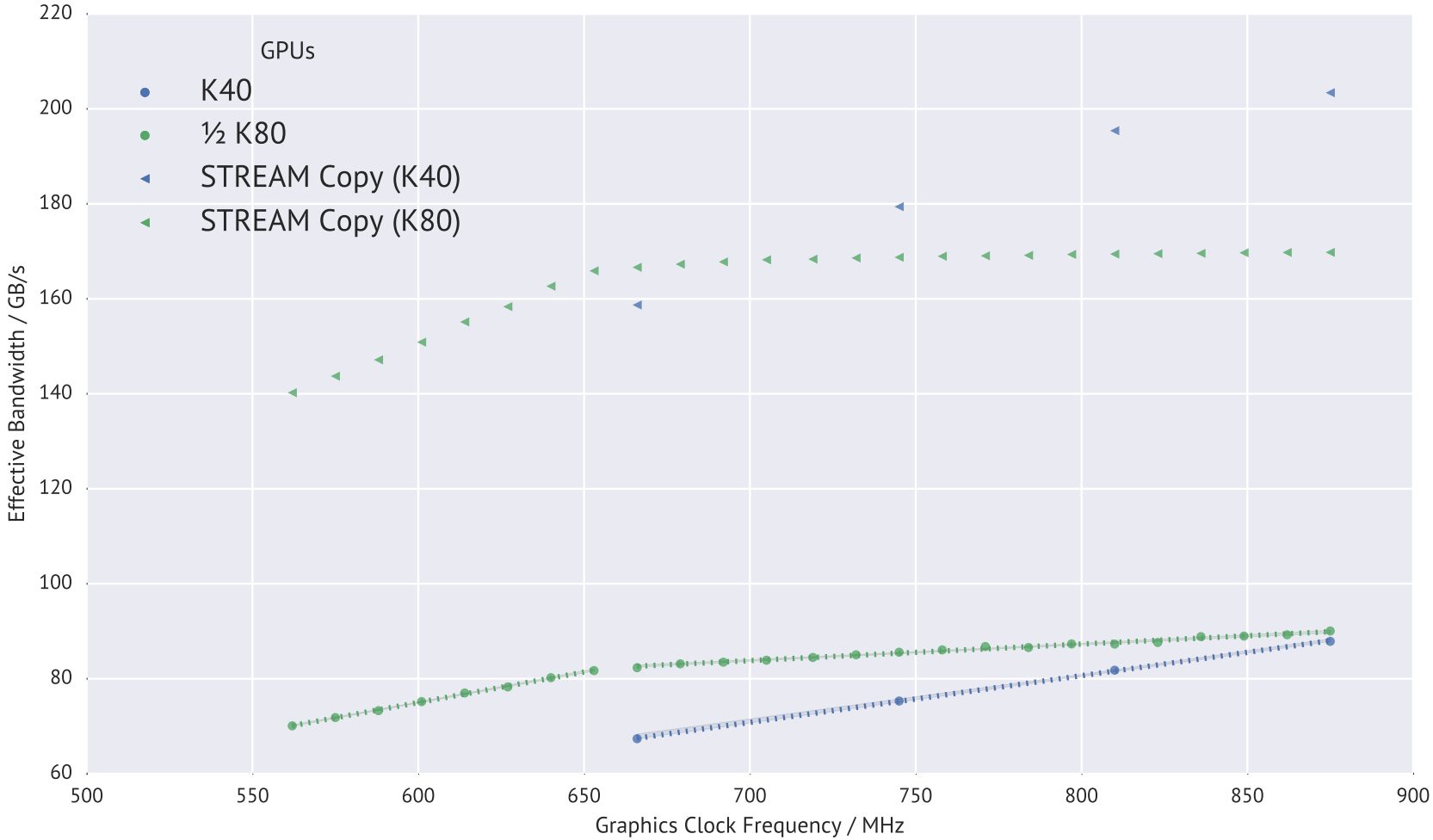


STREAM Bandwidth

As a means of normalization



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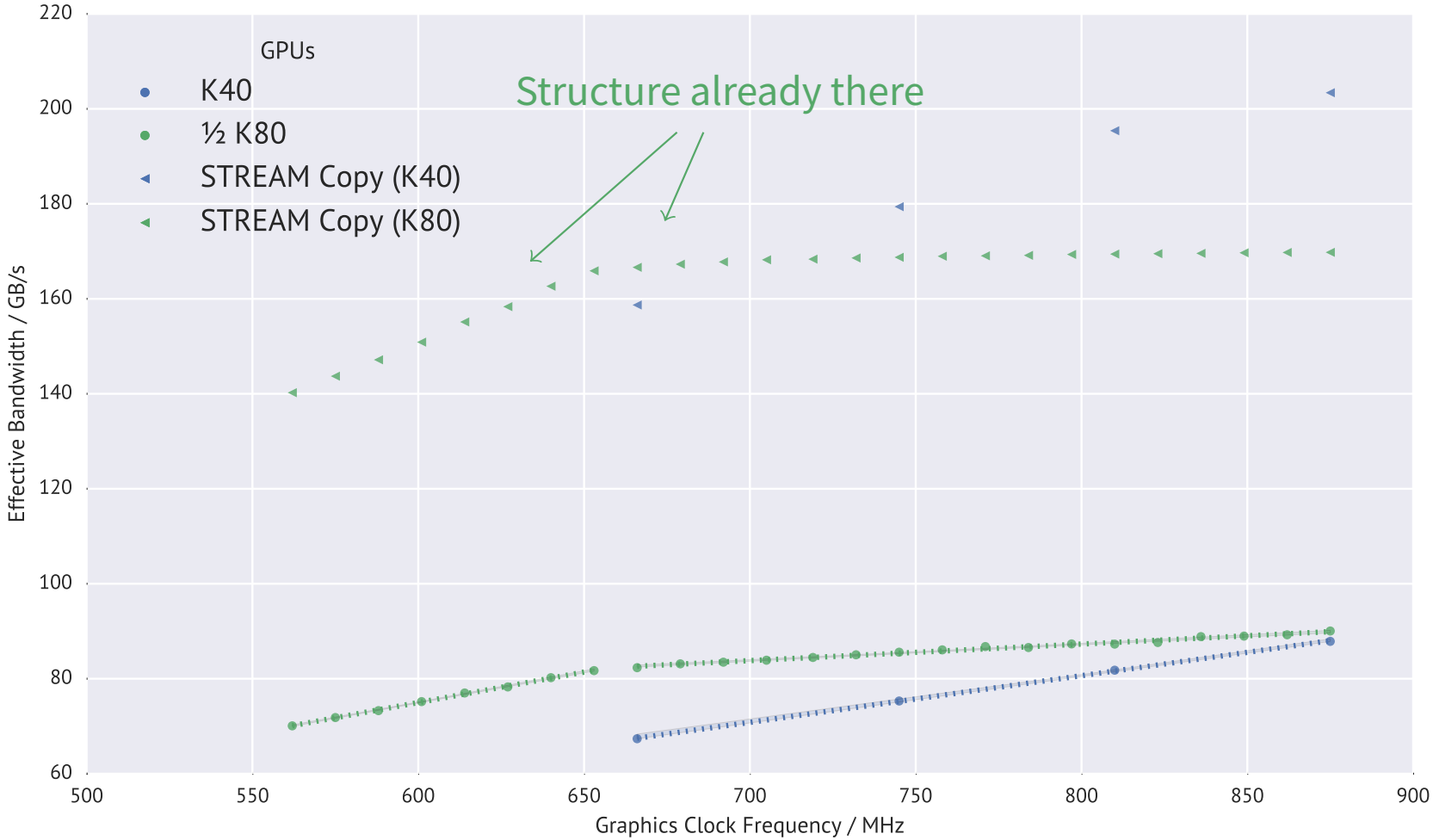
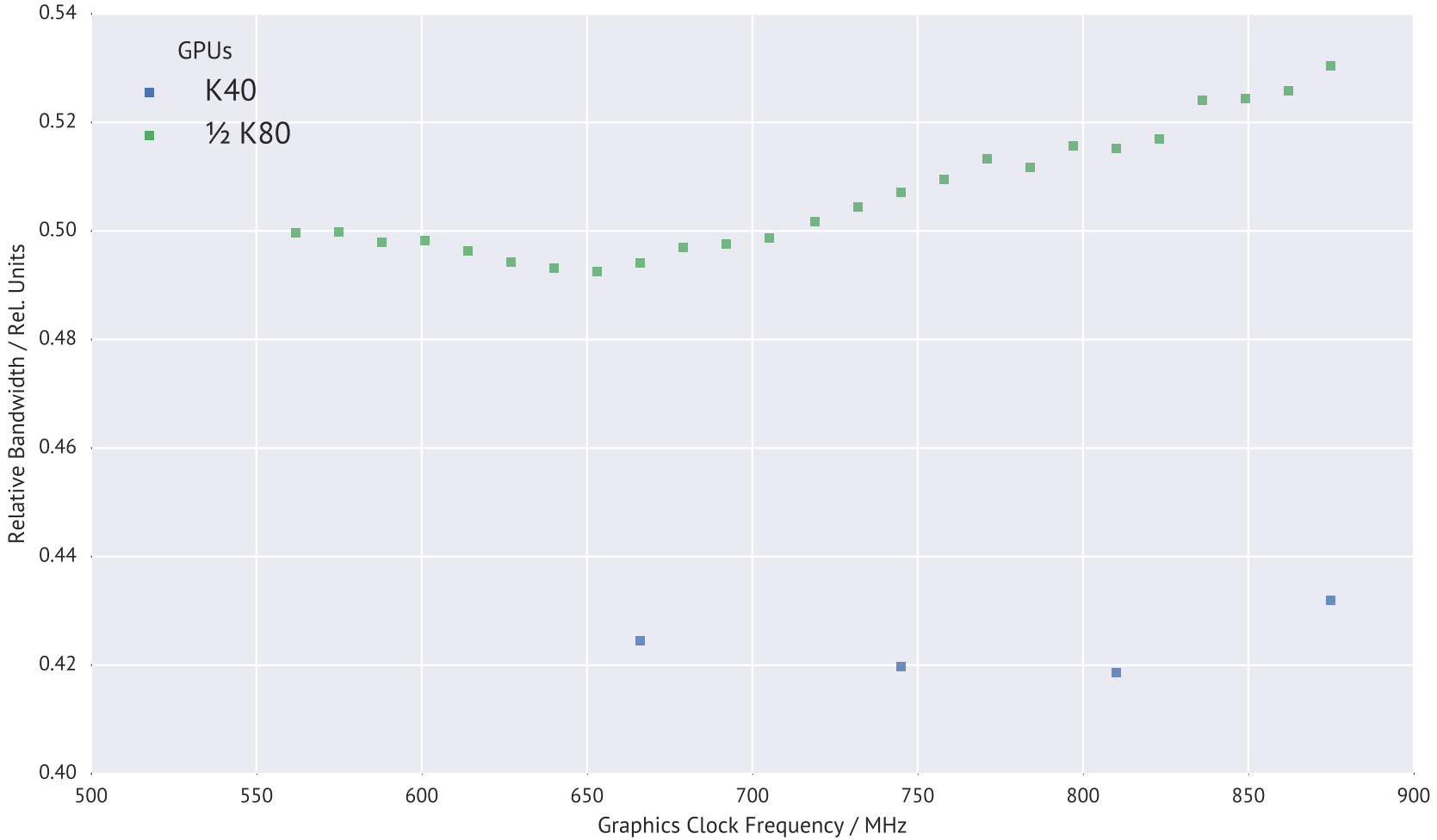


Normalized Clock-dependent Bandwidth

Bandwidth vs. Clock Frequency, normalized to STREAM results



Results & Conclusions

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- Performance Model
  - — Information exchange model: JuSPIC not bandwidth-limited
  - → Further investigation needed (Computation? **Latency?**)
  - — Peculiar: steps in STREAM (K80); *valley of efficiency* (K80, K40)
  - — More byte per clock cycle for ½K80 (before step)

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  - — JuSPIC's Fortran too complicated for OpenACC (7 bugs with PGI …)
  - — CUDA Fortran also portable, closer to original code
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  - — ½ of computing-heavy functions ported; promising results
  - ⇒ Full effect only if H↔D copies reduced → NVLink!

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Thank you for your attention!

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