Towards Exascale Computing with the Atmospheric Model NUMA

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- **NUMA** = **N**on-hydrostatic **U**nified **M**odel of the **A**tmosphere
- dynamical core inside the Navy's next generation weather prediction system NEPTUNE (**N**avy's **E**nvironment **P**rediction sys**T**em **U**sing the **N**uma **E**ngine)
- developed by **Prof. Francis X. Giraldo** and generations of postdocs

Goal

- **NOAA: HIWPP project plan: Goal for 2020:**
  ~ 3km – 3.5km global resolution within operational requirements

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  double precision, no shallow atmosphere approx., arbitrary terrain, IMEX in the vertical

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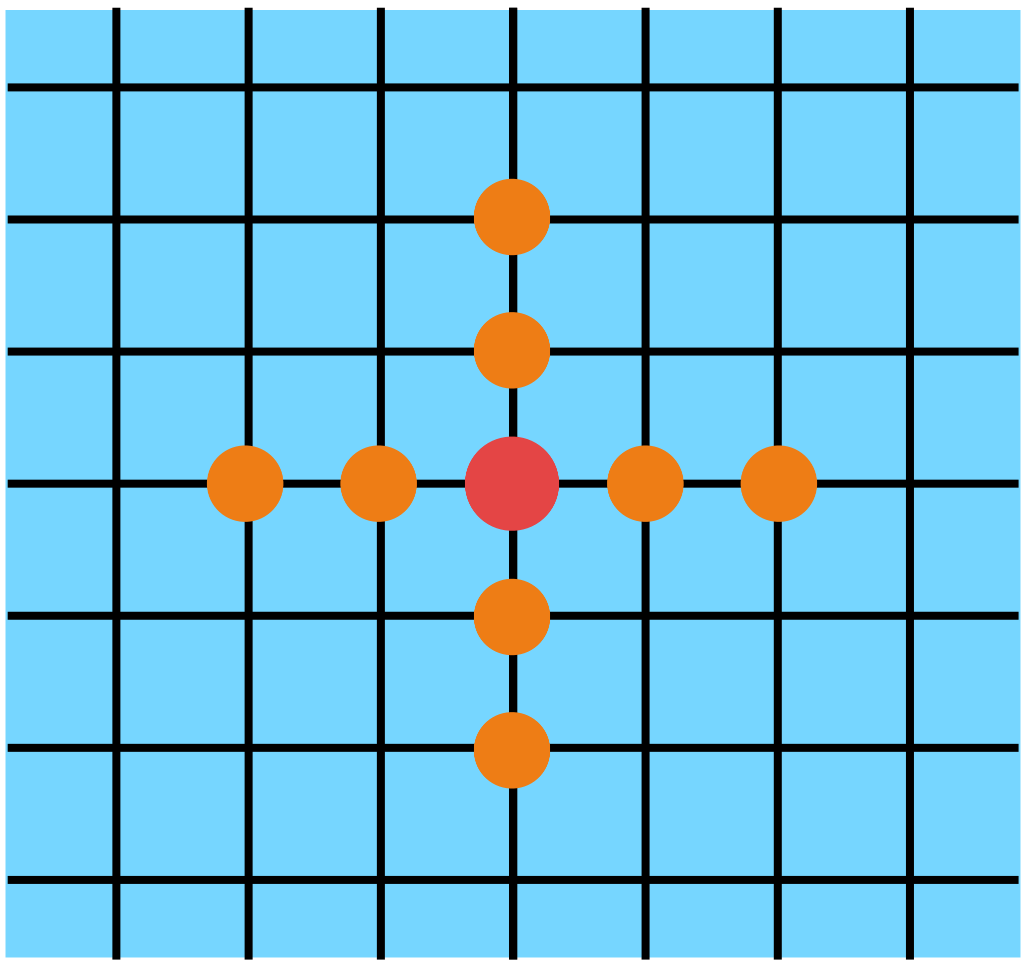
  double precision, no shallow atmosphere approx., arbitrary terrain, IMEX in the vertical

- **Expect:** 2km by doing more optimizations

Communication between processors

4th order Finite Difference



Communication between processors

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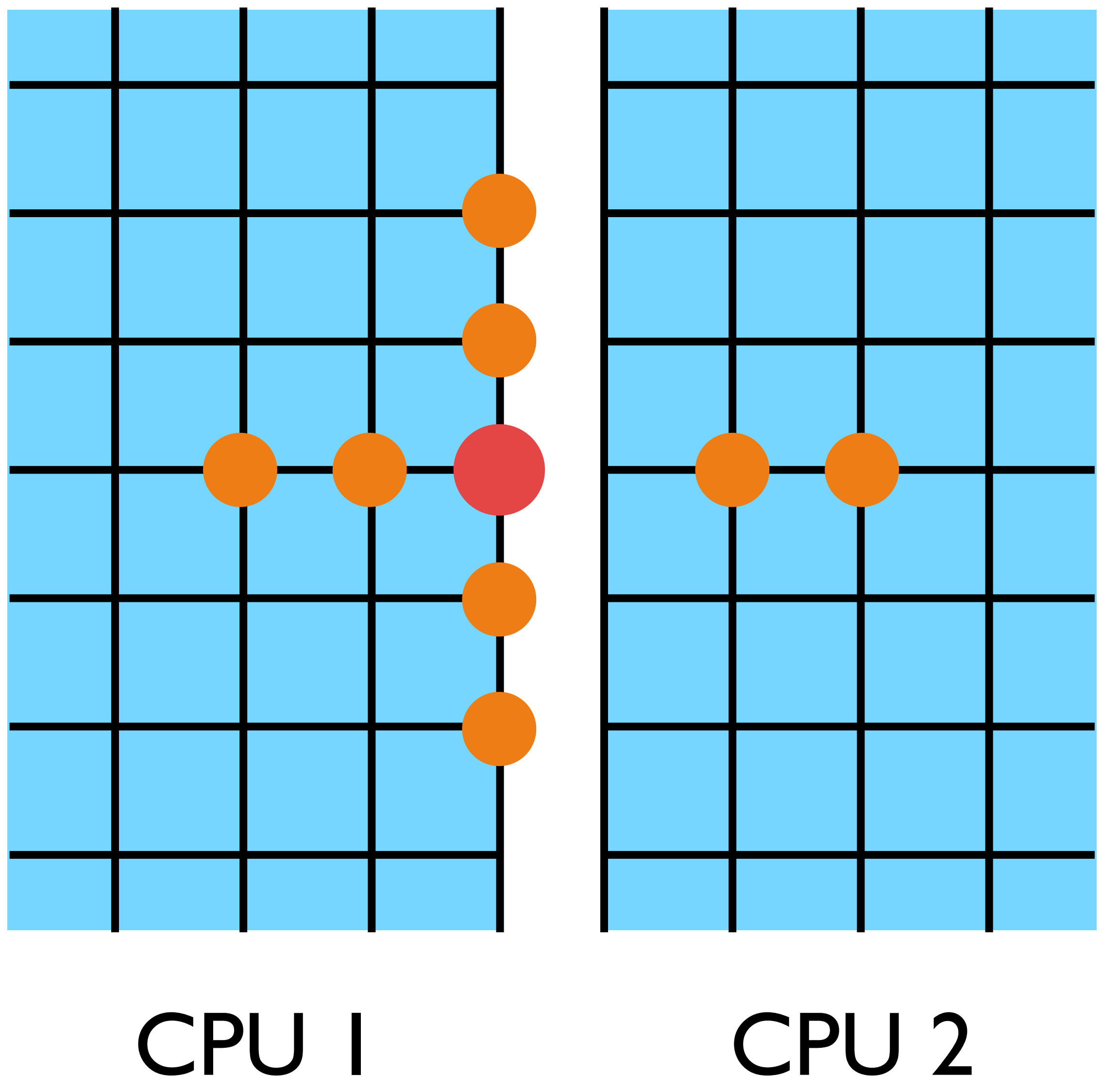

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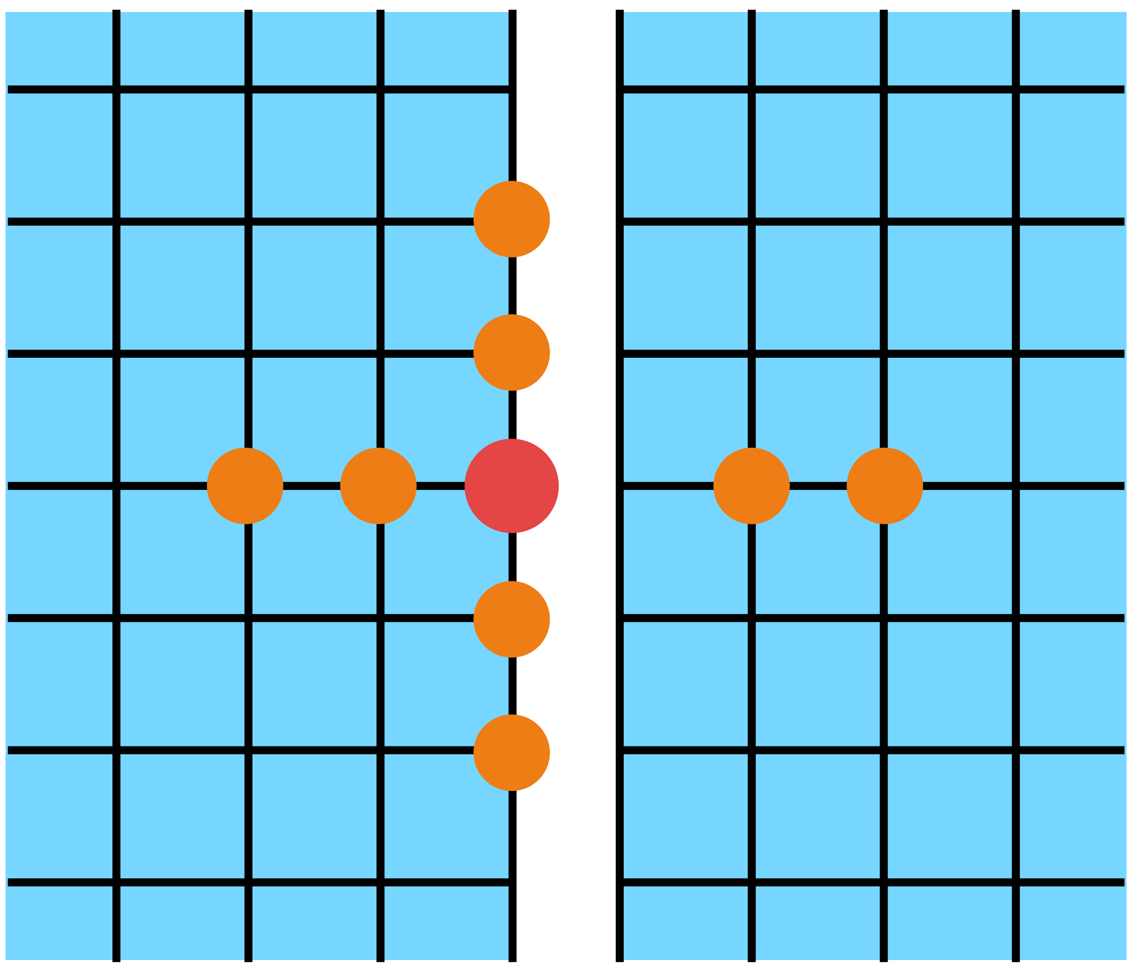
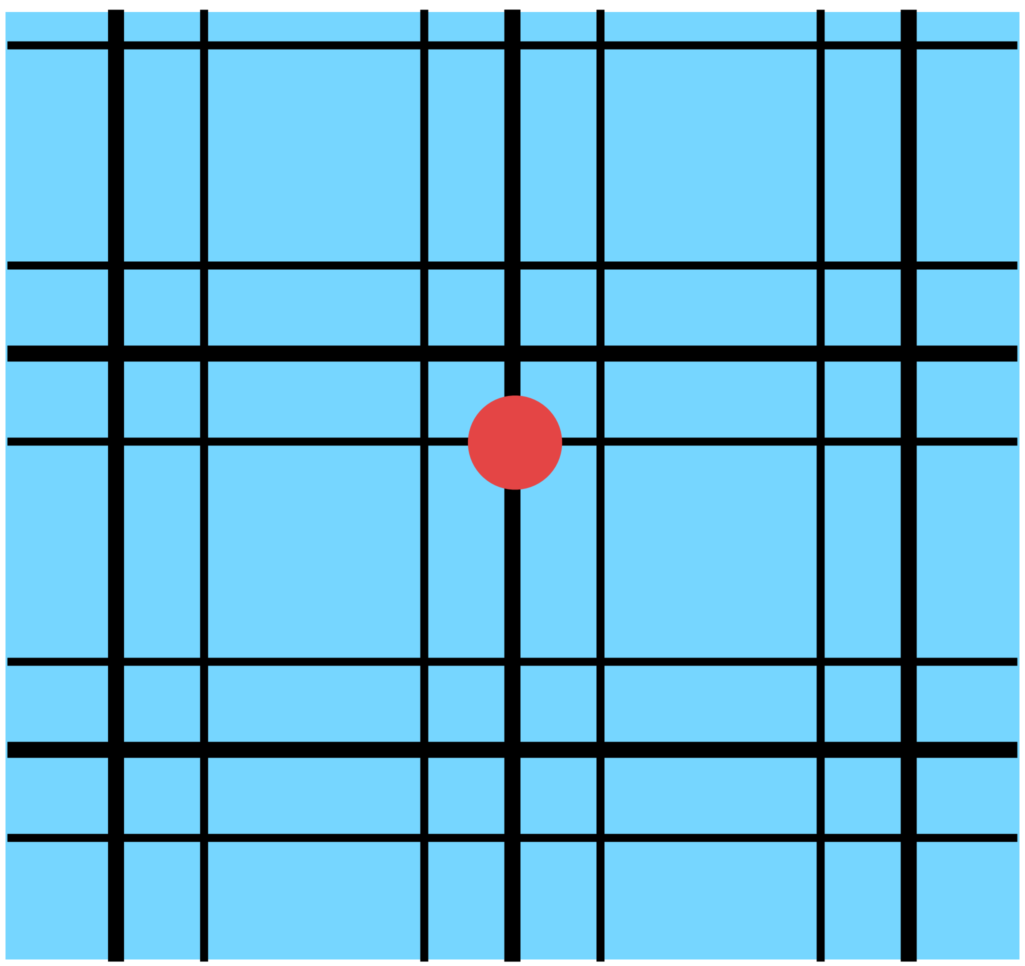


CPU 1 CPU 2

compact stencil methods (like in NUMA)



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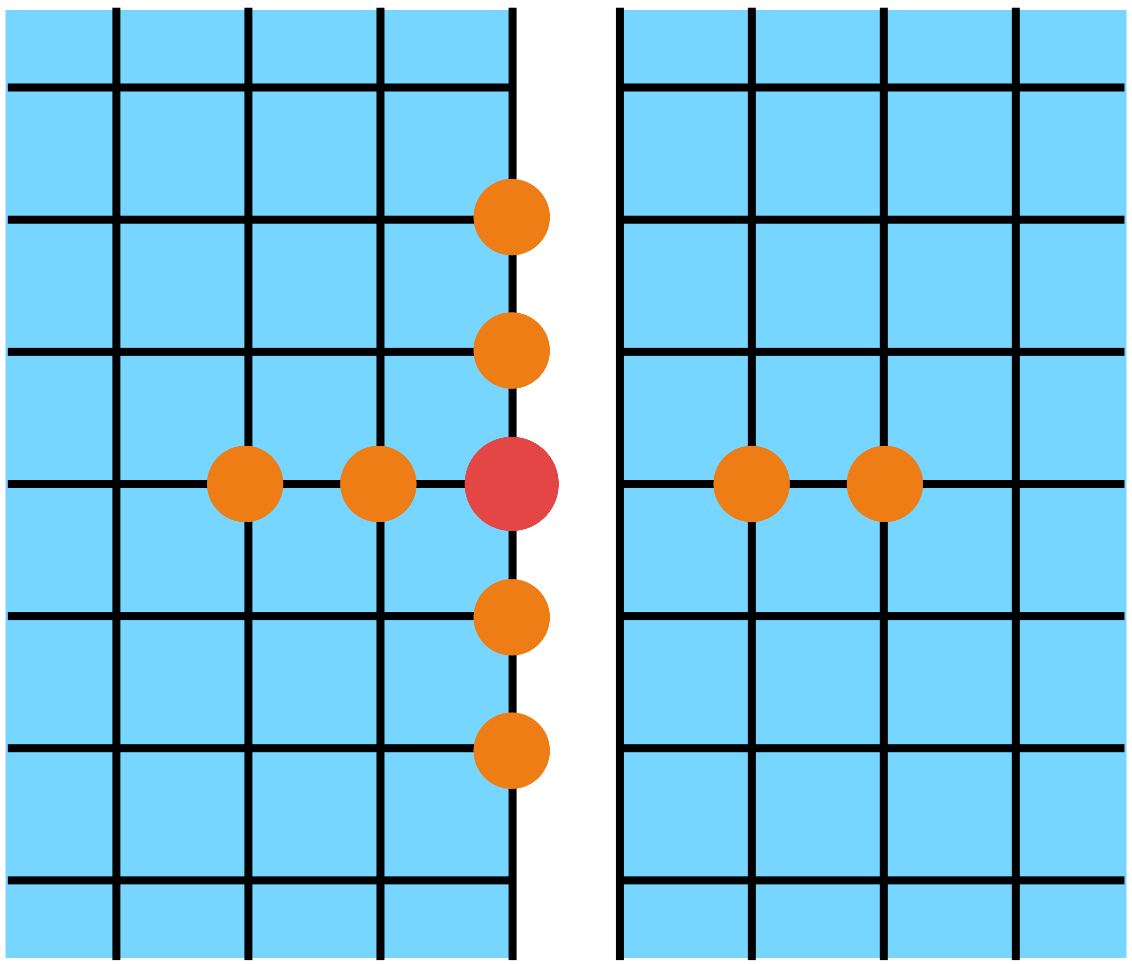

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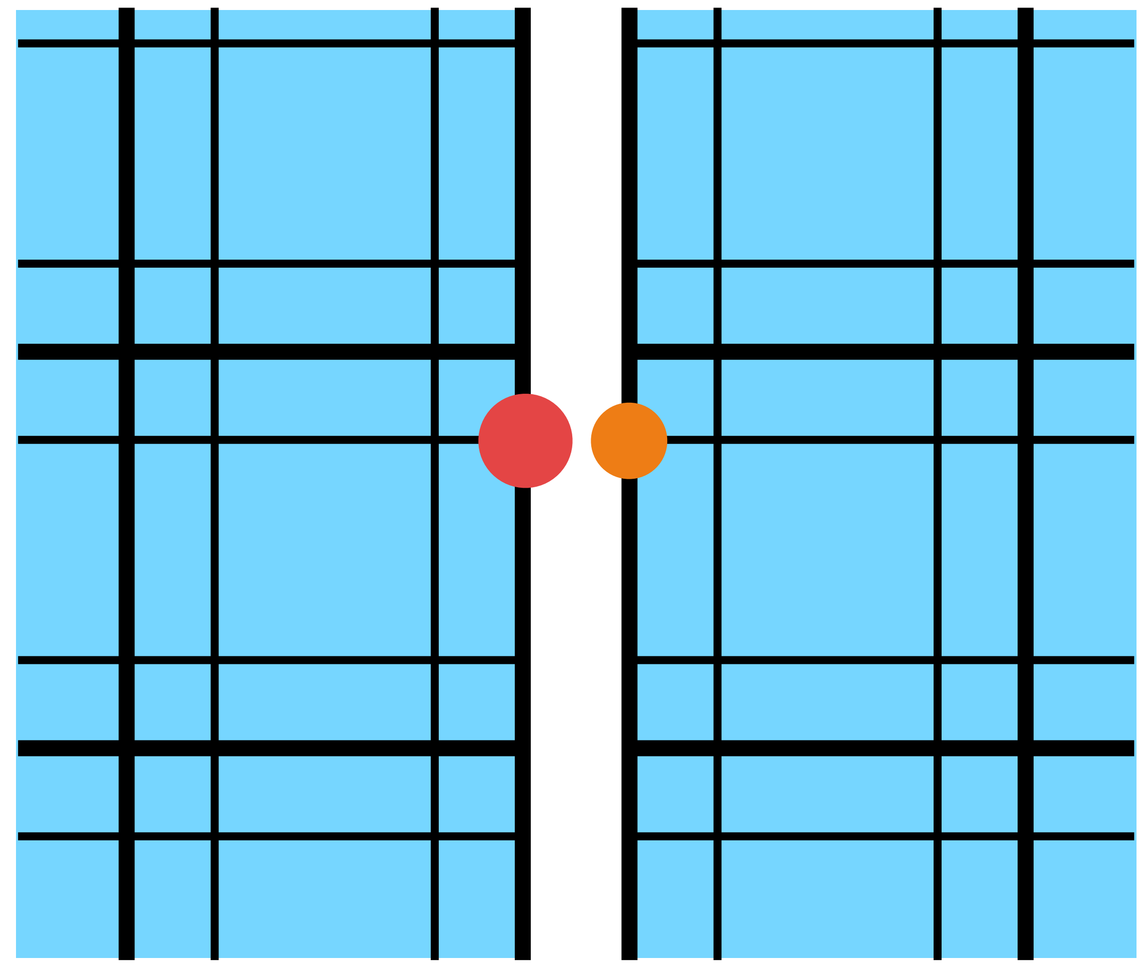

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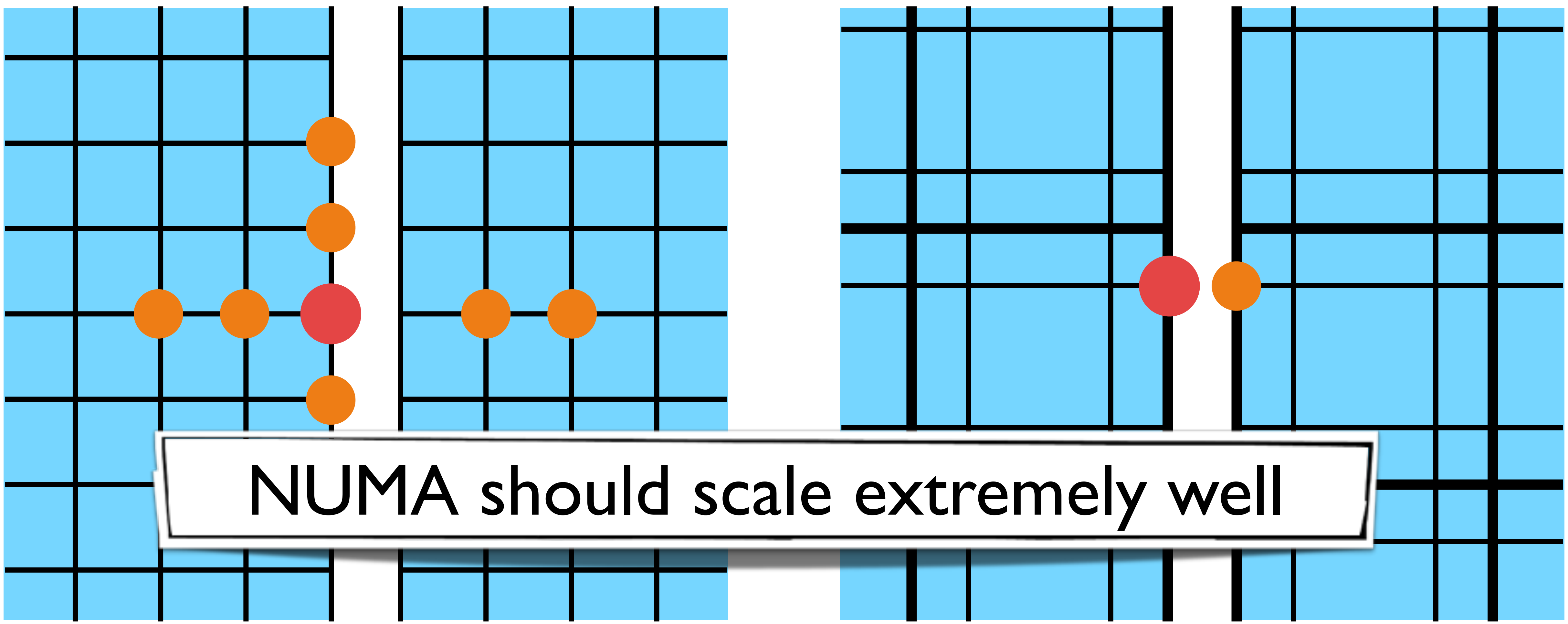

CPU 1 CPU 2 CPU 1 CPU 2

Fastest Supercomputers of the World
according to top500.org

#	NAME	COUNTRY	TYPE	PEAK (PFLOPS)
1	TaihuLight	China	Sunway	125.4
2	Tianhe-2	China	Intel Xeon Phi	54.9
3	Titan	USA	NVIDIA GPU	27.1
4	Sequoia	USA	IBM BlueGene	20.1
5	K computer	Japan	Fujitsu CPU	11.2
6	Mira	USA	IBM BlueGene	10.0

1 PFlops = 10^{15} floating point ops. per sec.

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overview

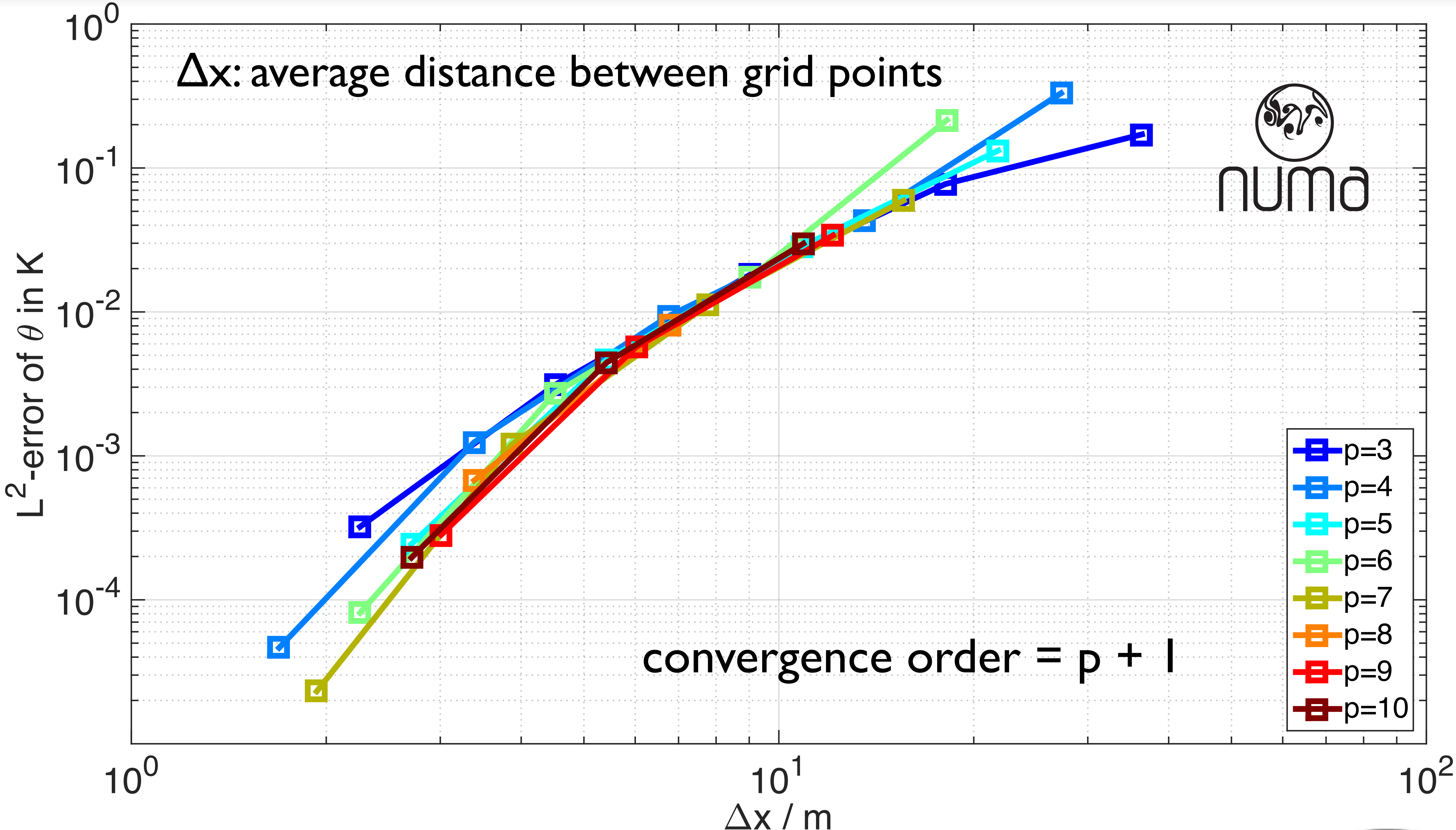
- Mira: Blue Gene
  strategy: optimize one setup for one specific computer
- Titan: GPUs
  strategy: keep all options, portability on CPUs and GPUs
- Intel Knights Landing

Mira: Blue Gene

optimize one setup for this specific computer

Which convergence order to use?

L2-error of pot. temperature for 2D rising bubble with viscosity μ=0.1m^2/s



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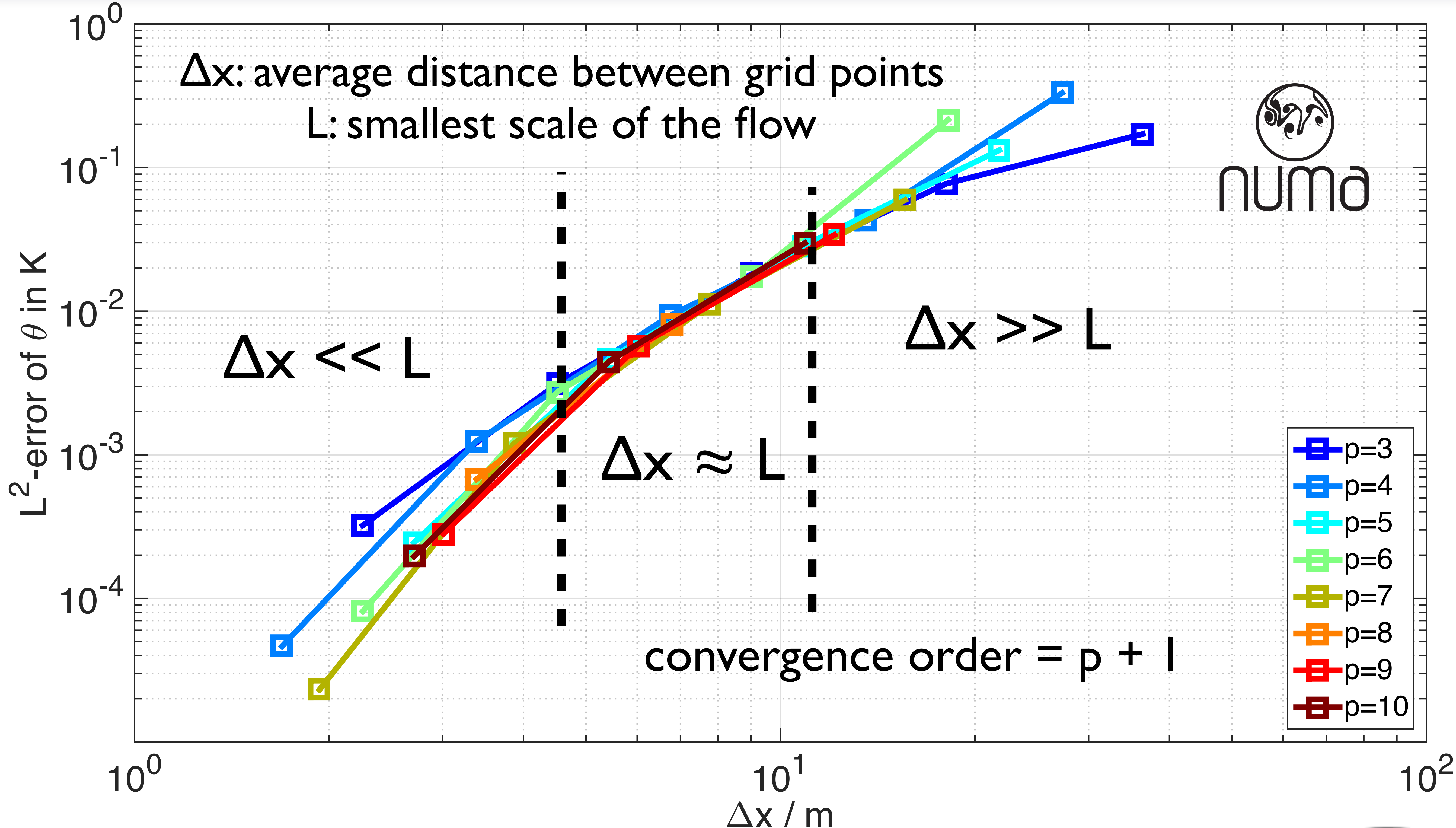

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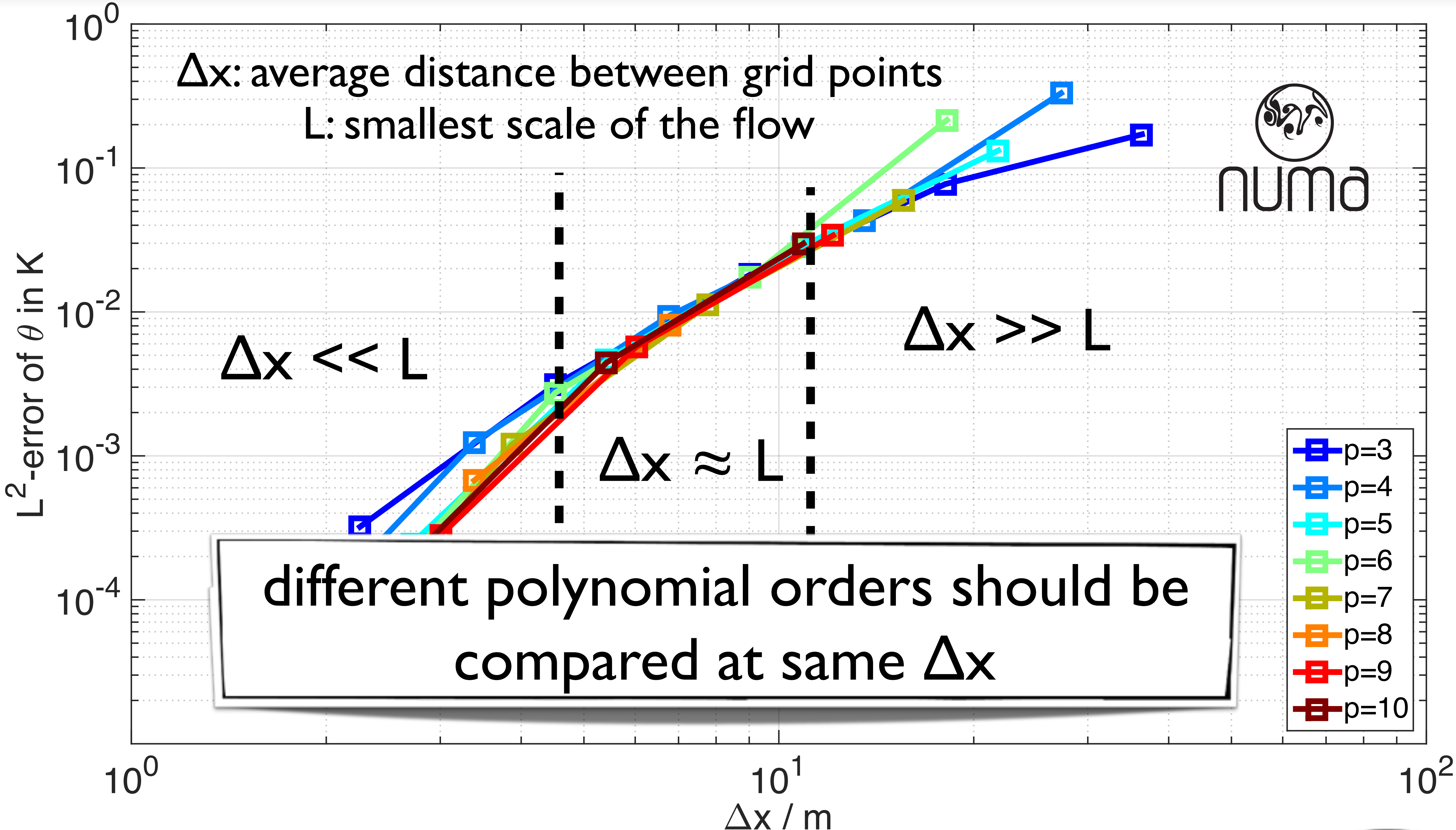
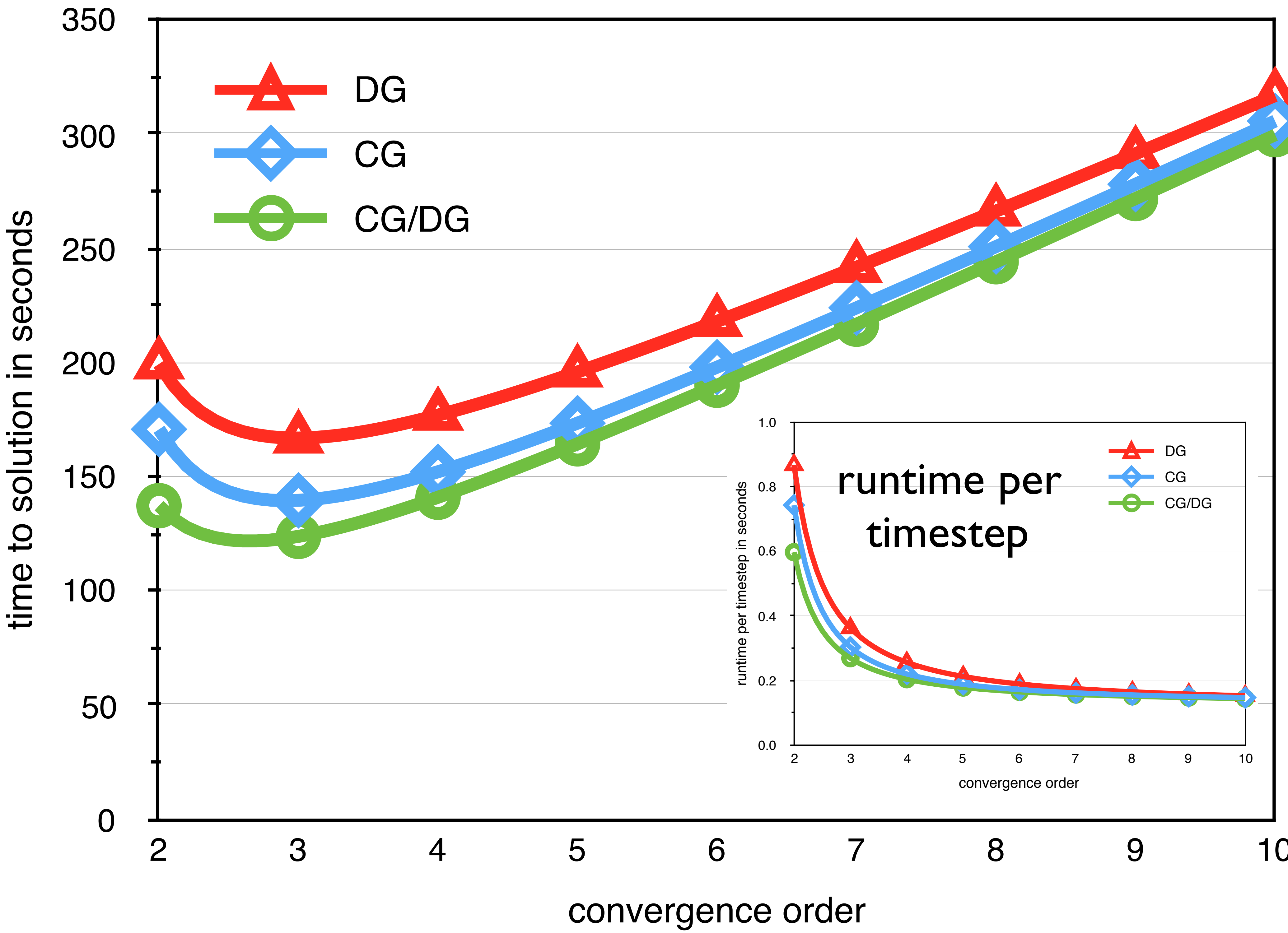


Which convergence order to use?

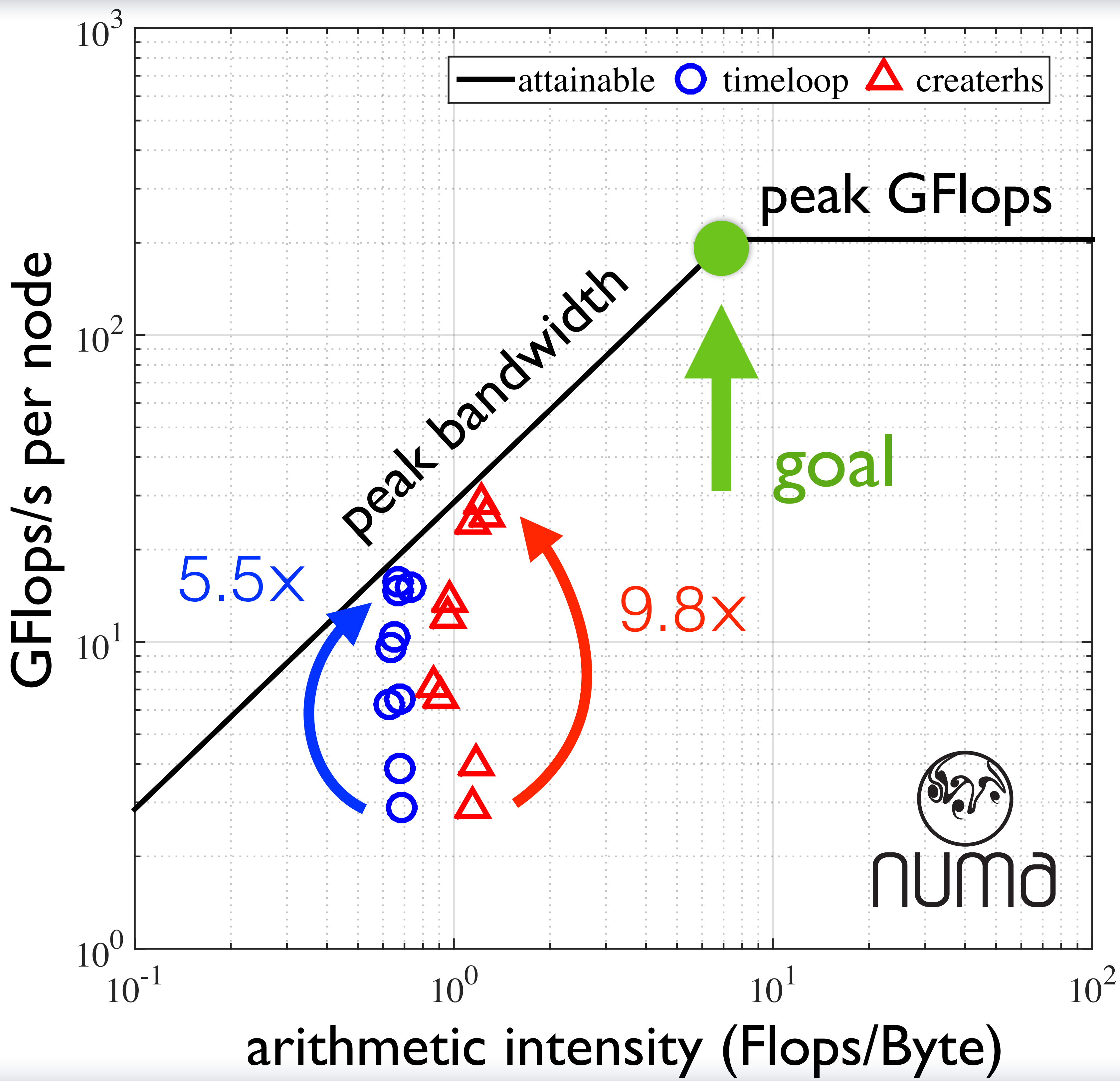
theoretical performance model for fixed Δx



Mira Titan KNL

Measurements: roofline plot

rising bubble test case on Mira



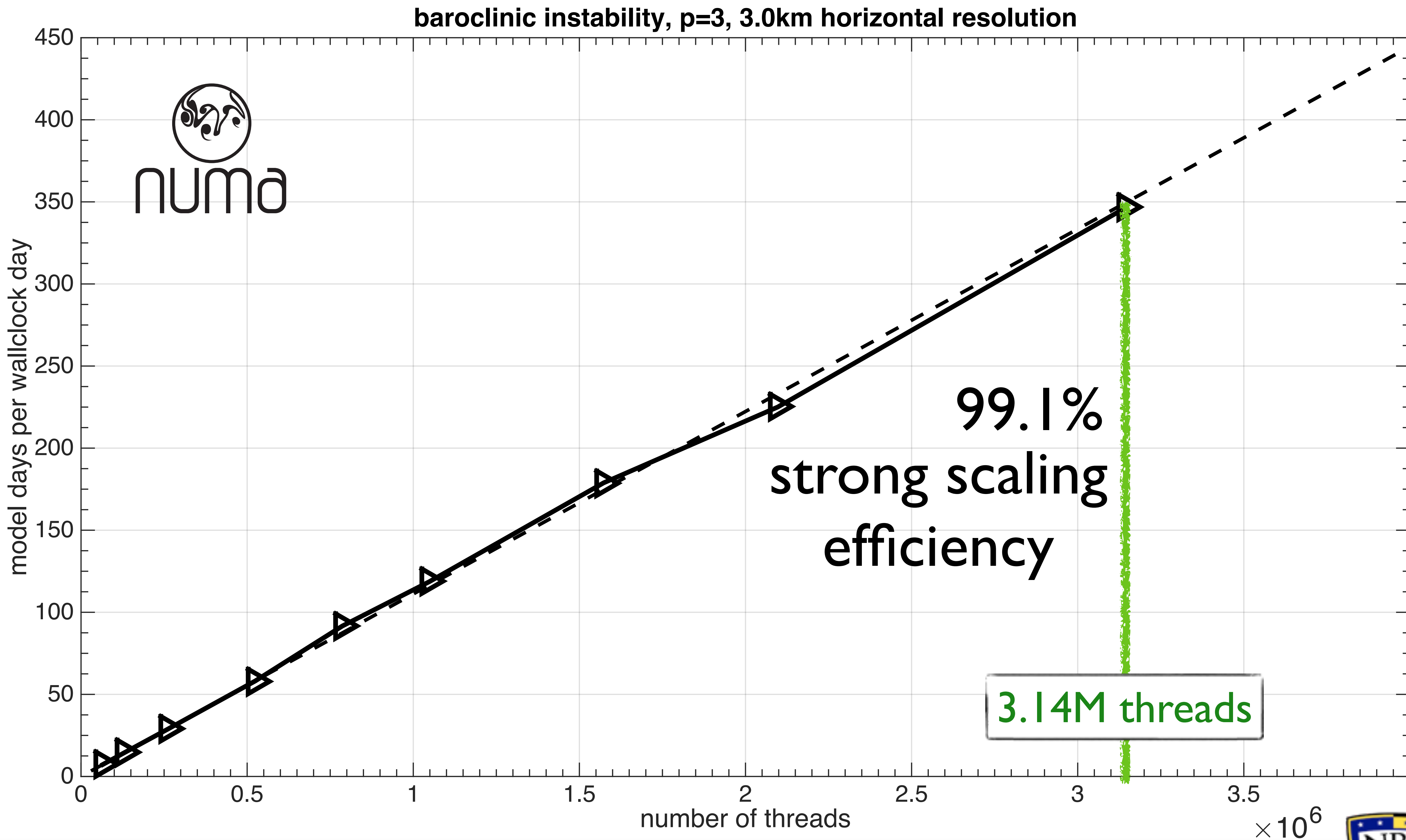
blue: entire timeloop

red: main computational kernel

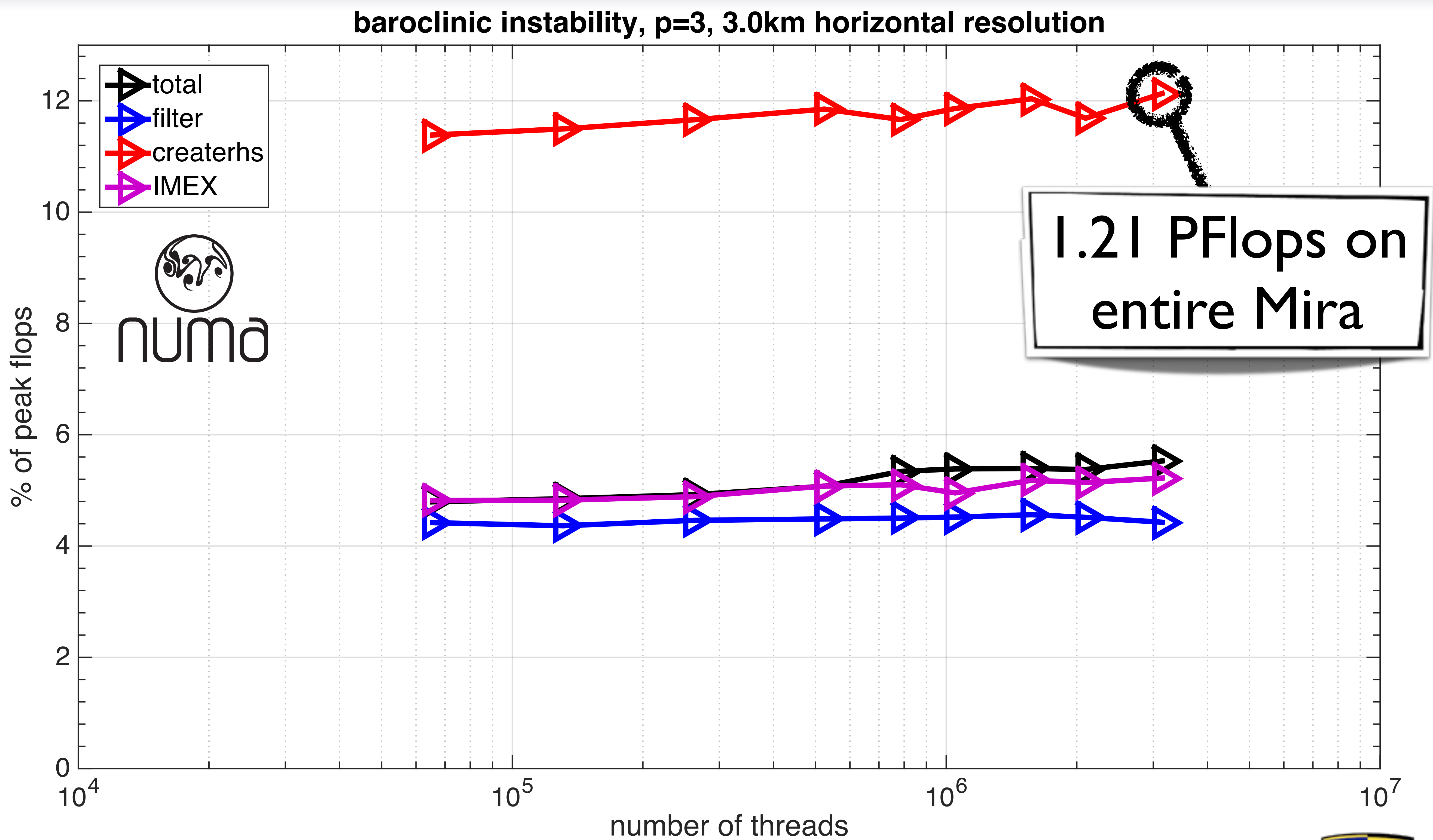
data points: different optimization stages

Strong scaling with NUMA

1.8 billion grid points (3.0km horizontal, 31 levels vertical)

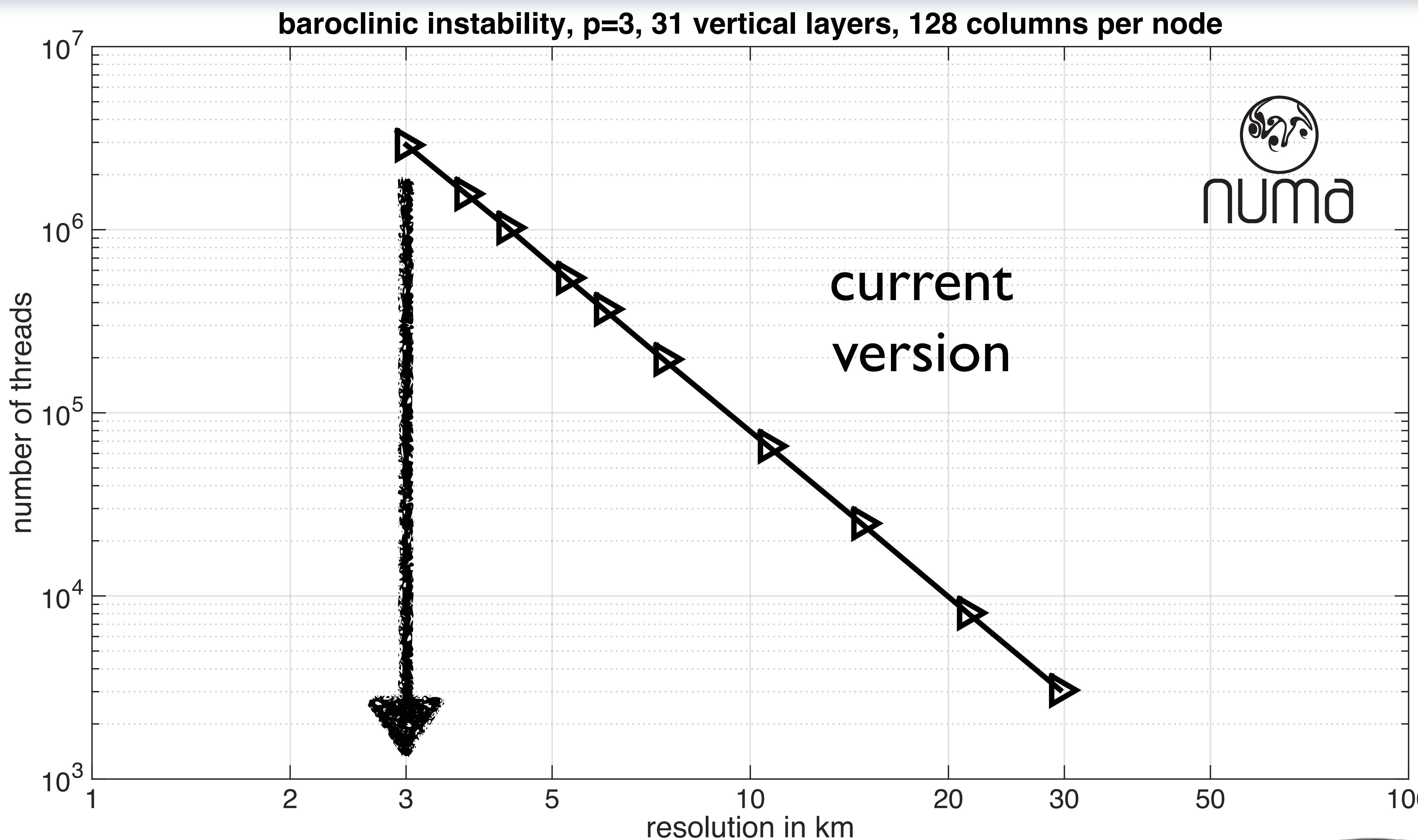


12.1% of theoretical peak (flops)



Where are we heading?

dynamics within 4.5 minutes runtime per one day forecast



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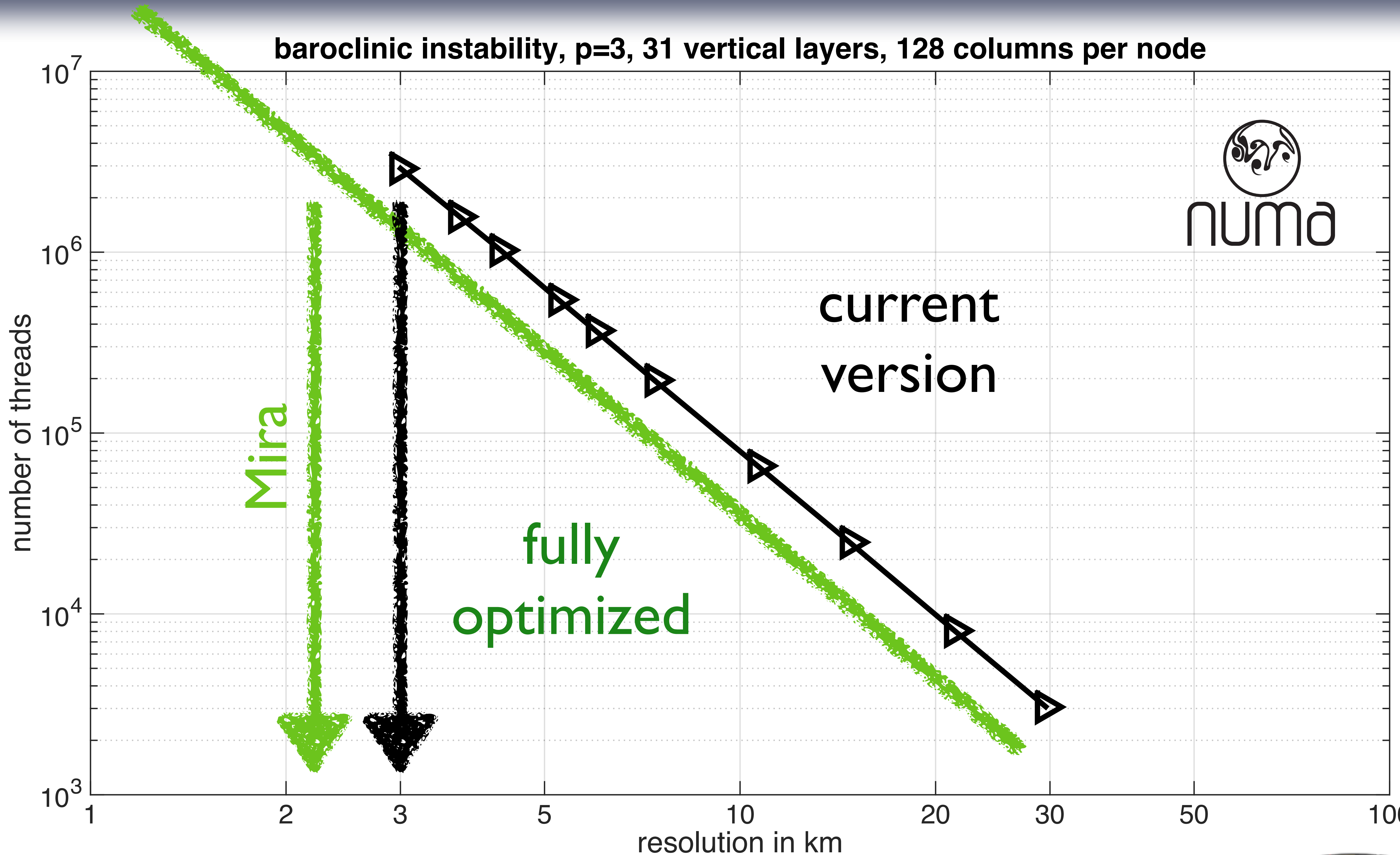

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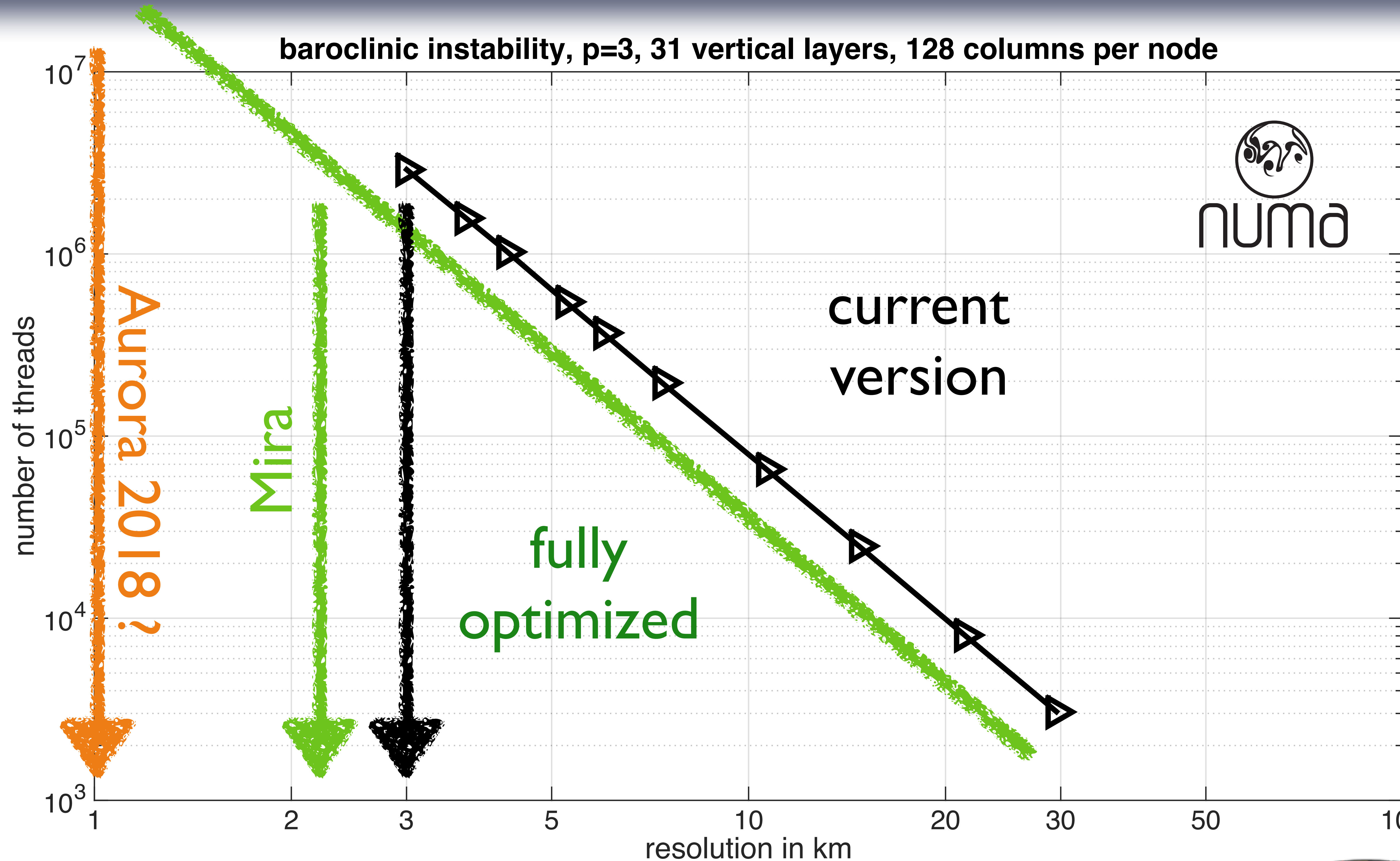


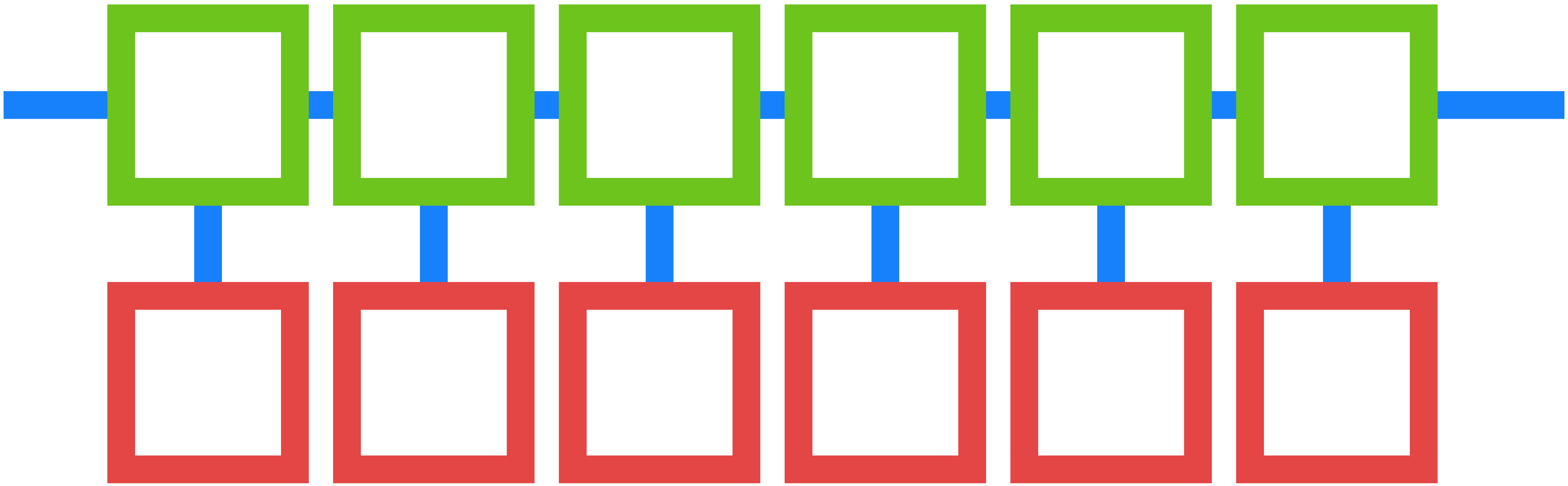
Titan: GPUs

keep all options, portability on CPUs and GPUs

Titan

18,688 CPU nodes
(16 cores each)

network

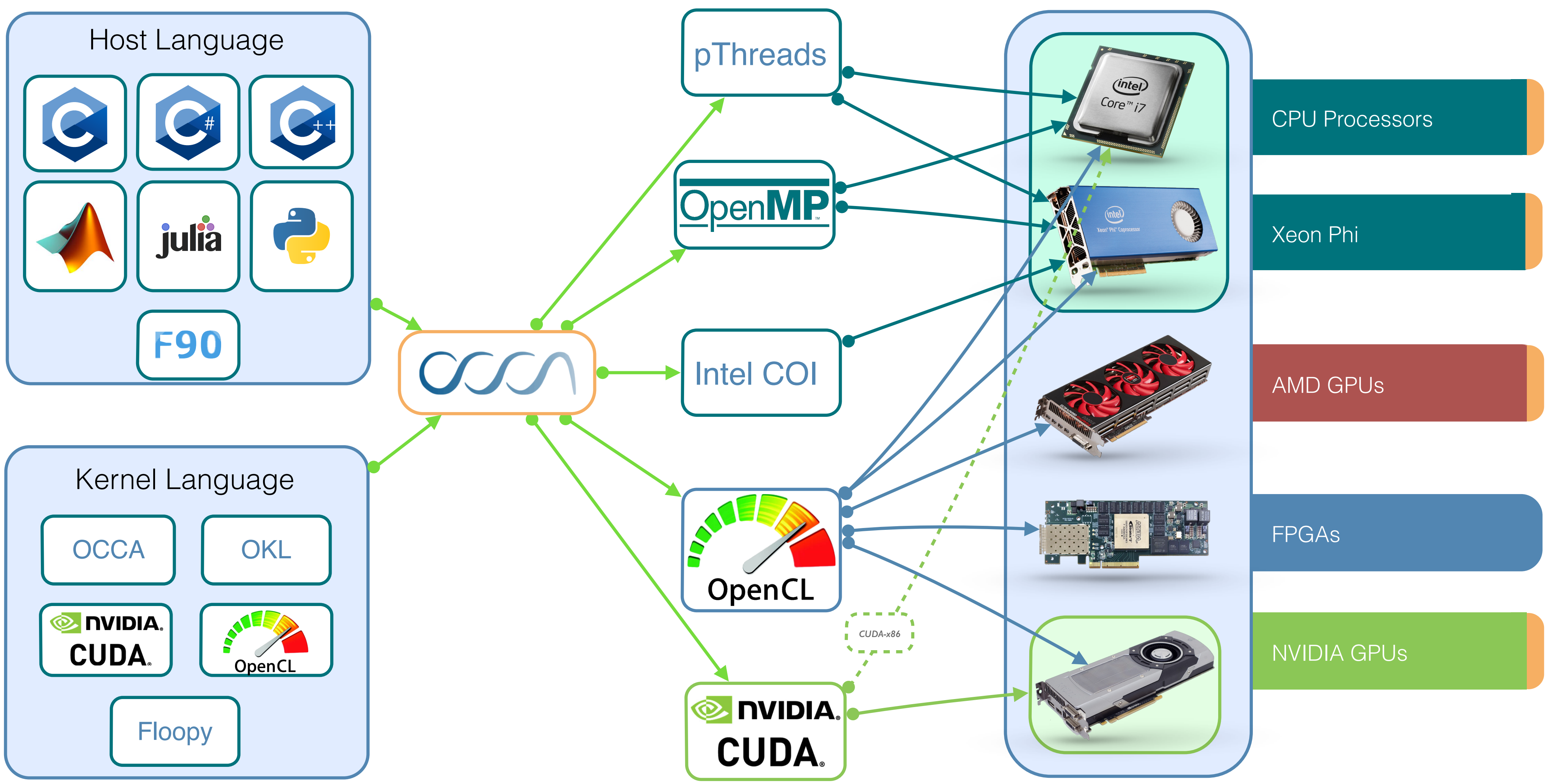


18,688 NVIDIA GPUs
(2,688 CUDA cores each)

OCCA2: unified threading model

(slide: courtesy of Lucas Wilcox and Tim Warburton)

Portability & extensibility: device independent kernel language (or OpenCL / CUDA) and native host APIs.



Available at: `https://github.com/tcew/OCCA2`

Floopy/OCCA2 code

(slide: courtesy of Lucas Wilcox and Tim Warburton)

```
allocate(a(1:entries), b(1:entries), ab(1:entries), stat = alloc_err)
if (alloc_err /= 0) stop "*** Not enough memory ***"

do i=1,entries
  a(i) = i-1
  b(i) = 2-i
  ab(i) = 0
end do

device = occaGetDevice(mode, platformID, deviceID)

o_a  = occaDeviceMalloc(device, int(entries,8)*4_8)
o_b  = occaDeviceMalloc(device, int(entries,8)*4_8)
o_ab = occaDeviceMalloc(device, int(entries,8)*4_8)

addVectors = occaBuildKernelFromFloopy(device, "addVectors.floopy", "addVectors", "")

dims     = 1
innerDim = 16

call occaKernelSetAllWorkingDims(addVectors, dims, &
                                 int(innerDim,8), 1_8, 1_8, &
                                 int((entries + innerDim - 1)/innerDim,8), 1_8, 1_8)

call occaCopyPtrToMem(o_a, a(1), int(entries,8)*4_8, 0_8);
call occaCopyPtrToMem(o_b, b(1));

call occaKernelRun(addVectors, occaTypeMem_t(entries), o_a, o_b, o_ab)

call occaCopyMemToPtr(ab(1), o_ab);

print *,"a = ", a(:)
print *,"b = ", b(:)
print *,"ab = ", ab(:)

deallocate(a, b, ab, stat = alloc_err)
if (alloc_err /= 0) stop "*** deallocation not successful ***"
```

Floopy/OCCA2 code

(slide: courtesy of Lucas Wilcox and Tim Warburton)

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allocate(a(1:entries), b(1:entries), ab(1:entries), stat = alloc_err)
if (alloc_err /= 0) stop "*** Not enough memory ***"

do i=1,entries
  a(i) = i-1
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end do

device = occaGetDevice(mode, platformID, deviceID

o_a  = occaDeviceMalloc(device, int(entries,8)*4_
o_b  = occaDeviceMalloc(device, int(entries,8)*4_
o_ab = occaDeviceMalloc(device, int(entries,8)*4_

addVectors = occaBuildKernelFromFloopy(device, "a

dims     = 1
innerDim = 16

call occaKernelSetAllWorkingDims(addVectors, dims
                                 int(innerDim,8),
                                 int((entries + i

call occaCopyPtrToMem(o_a, a(1), int(entries,8)*4
call occaCopyPtrToMem(o_b, b(1));

call occaKernelRun(addVectors, occaTypeMem_t(entr

call occaCopyMemToPtr(ab(1), o_ab);

print *,"a = ", a(:)
print *,"b = ", b(:)
print *,"ab = ", ab(:)

deallocate(a, b, ab, stat = alloc_err)
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```

```
subroutine addVectors(entries, a, b, ab)
  implicit none

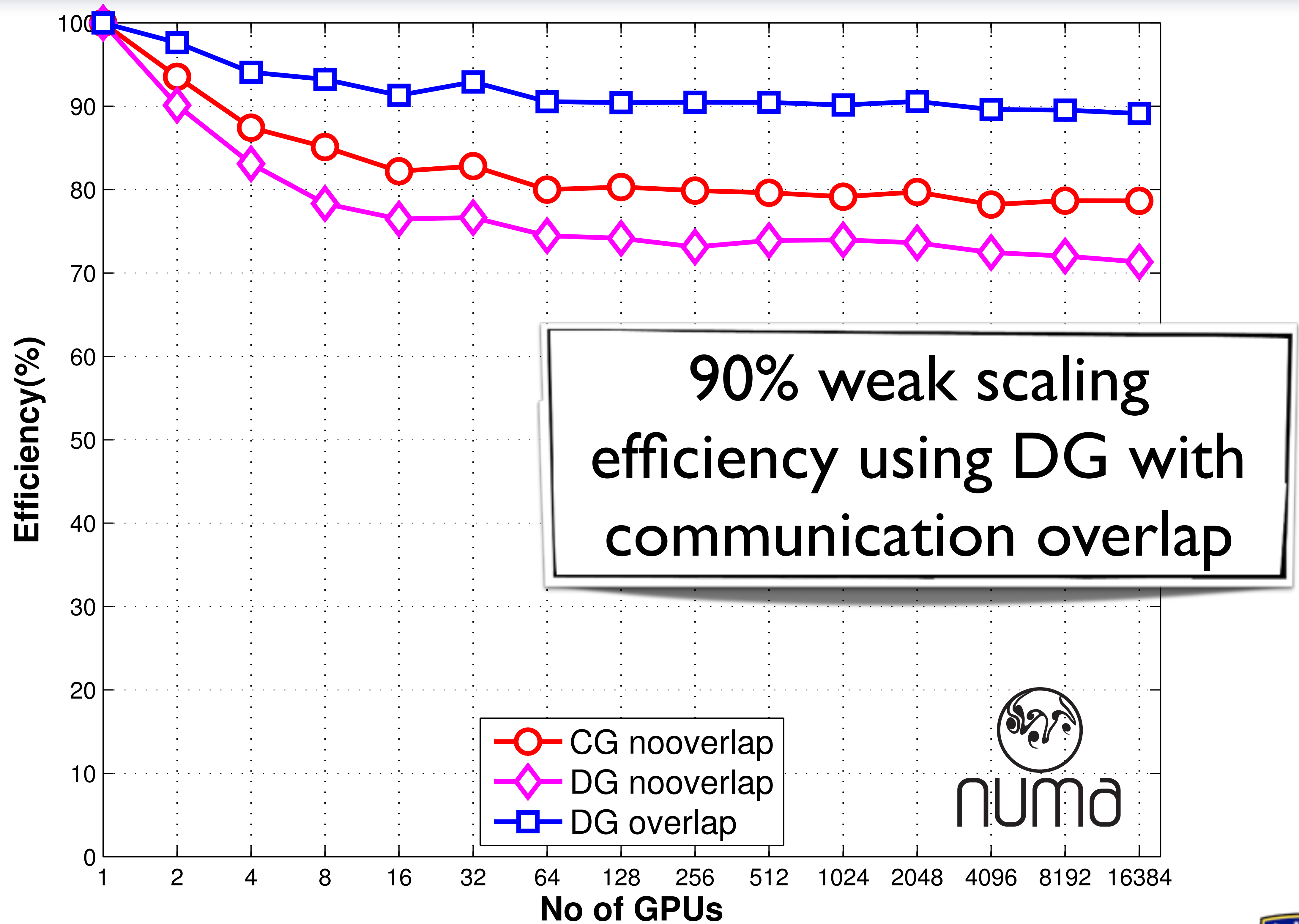
  integer*4 entries
  real*4 a(entries), b(entries), ab(entries)

  do i = 1, entries
    ab(i) = a(i) + b(i)
  end do
end

!$loopy begin transform
!
! addVectors = lp.split_iname(addVectors, "i", 16,
!     outer_tag="g.0", inner_tag="l.0")
!
!$loopy end transform
```

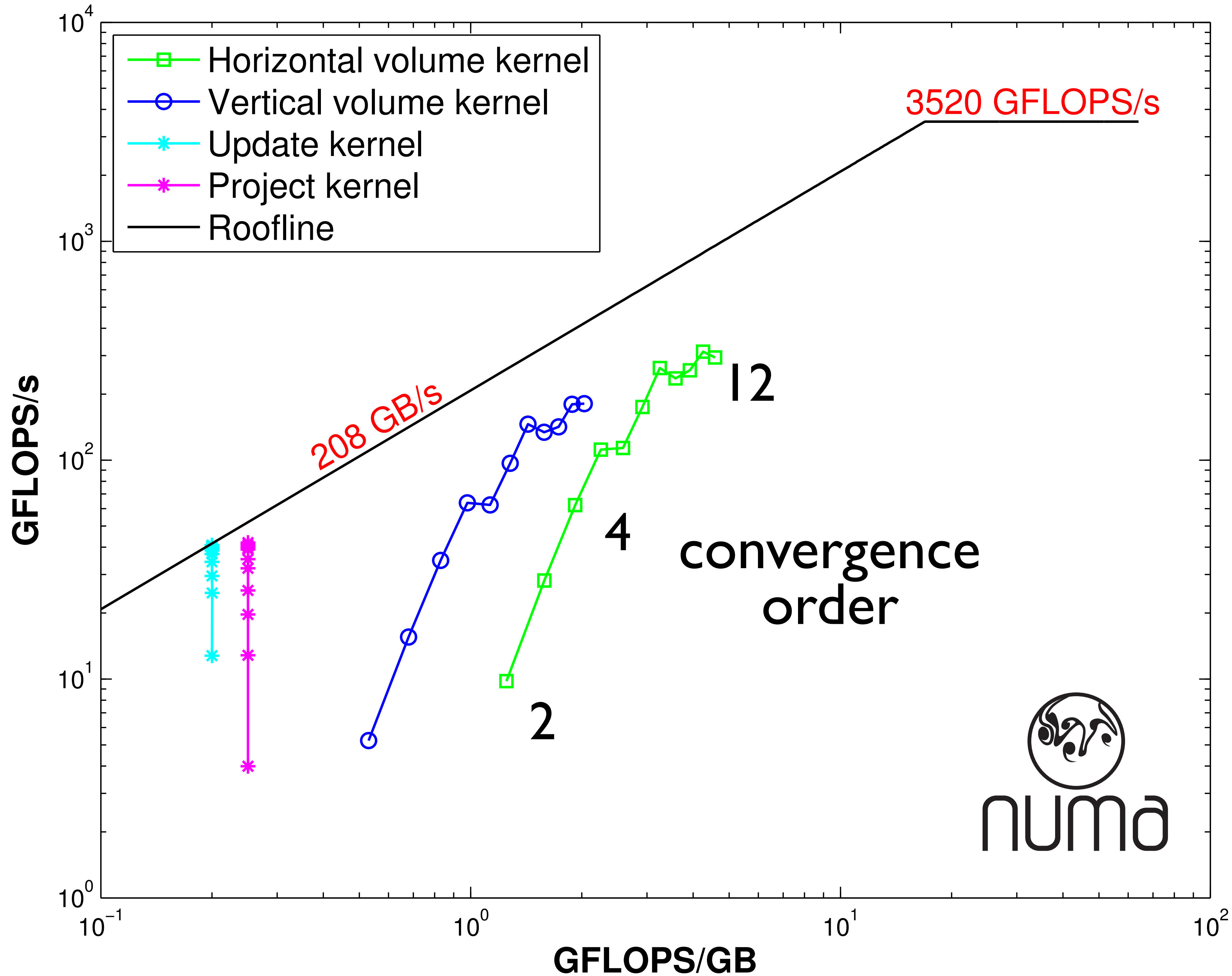
Weak scaling up to 16,384 GPUs (88% of Titan)

using 900 elements per GPU, polynomial order 8 (up to 10.7 billion grid points)



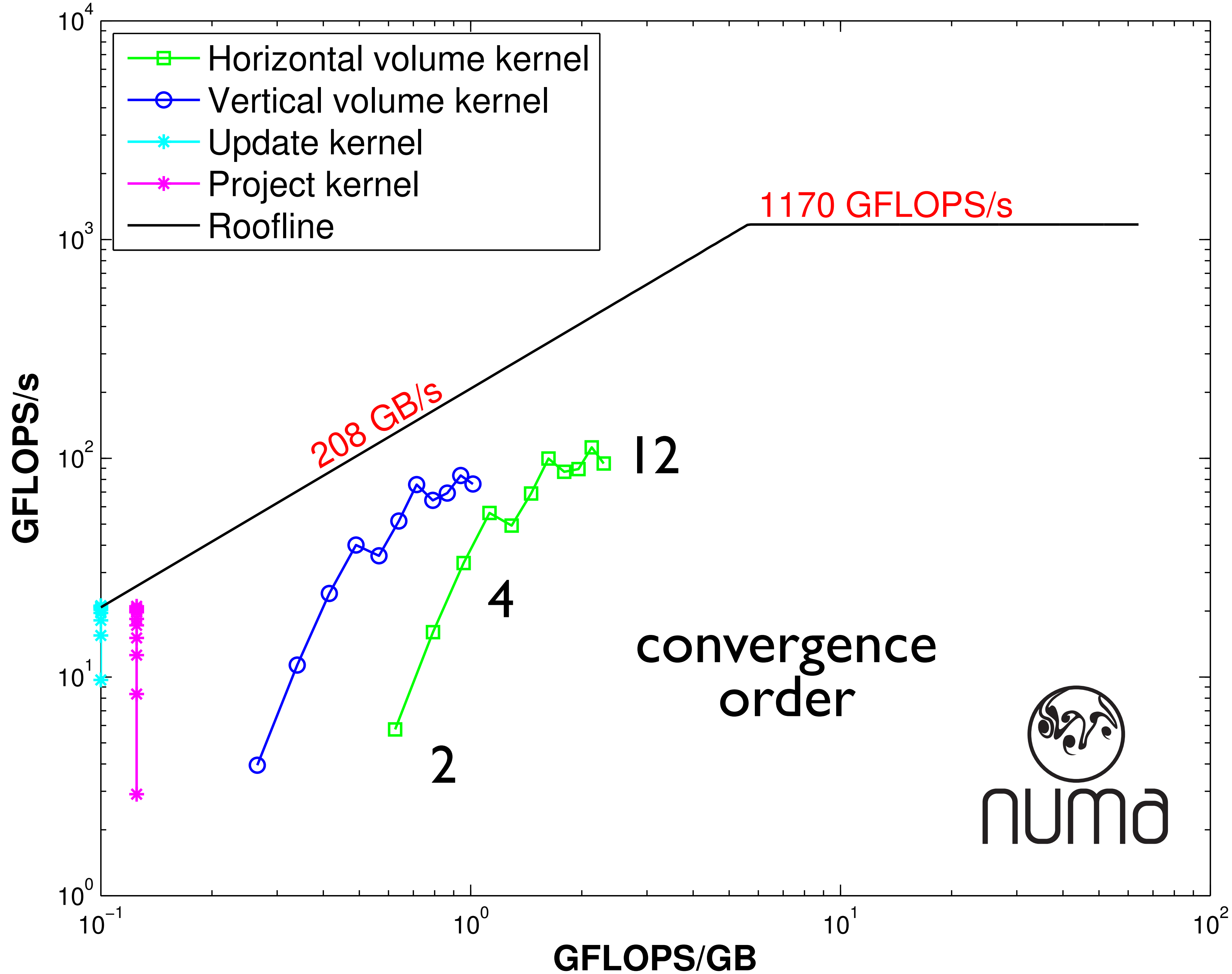
roofline plot: single precision

on the NVIDIA K20X GPU on Titan



roofline plot: double precision

on the NVIDIA K20X GPU on Titan



some more results from Titan

- GPU: up to 15 times faster than original version on one CPU node for single precision (CAM-SE and other models: less than 5x speed-up)

- CPU: single precision about 30% faster than double

- GPU: single about 2x faster than double

	CPU node	GPU
	16-core AMD Opteron 6274	NVIDIA K20X
peak performance	141 GFlops/s	1.31 TFlops/s
peak bandwidth	32 GB/s	208 GB/s
peak energy	115 W	235 W

Intel Knights Landing

Knights Landing

Why is this so exciting?

- 64 cores (Mira: 64 hardware threads)
- each Knights Landing chip has 16GB MCDRAM with 440GB/s memory bandwidth

$\Rightarrow$ more than 15 times faster than Mira

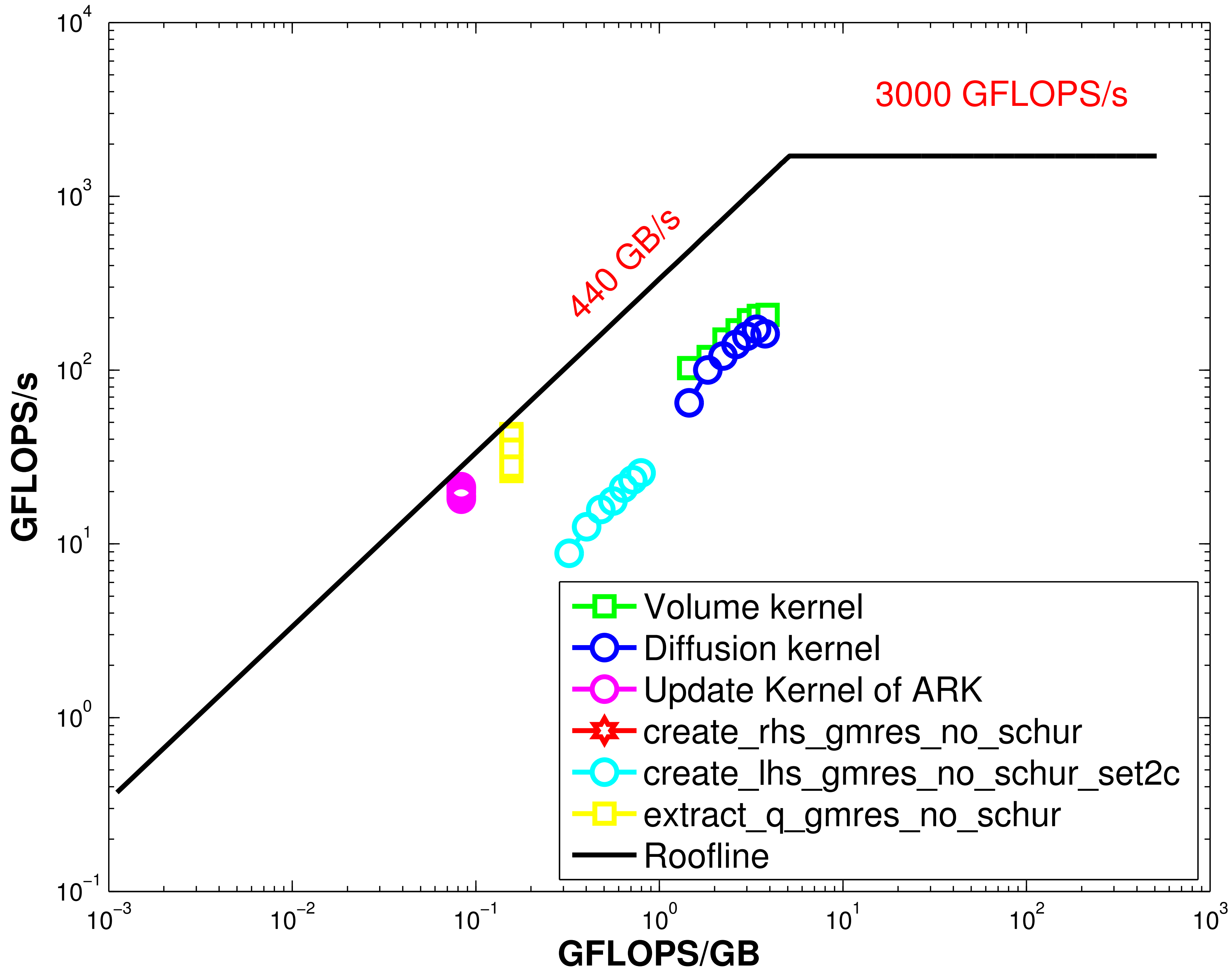
- Aurora (successor of Mira, expected in 2018): more than 50k Knights Landing nodes

$\Rightarrow$ more nodes than Mira

- overall: Aurora should allow us to run the same simulations like on Mira but 15 times faster

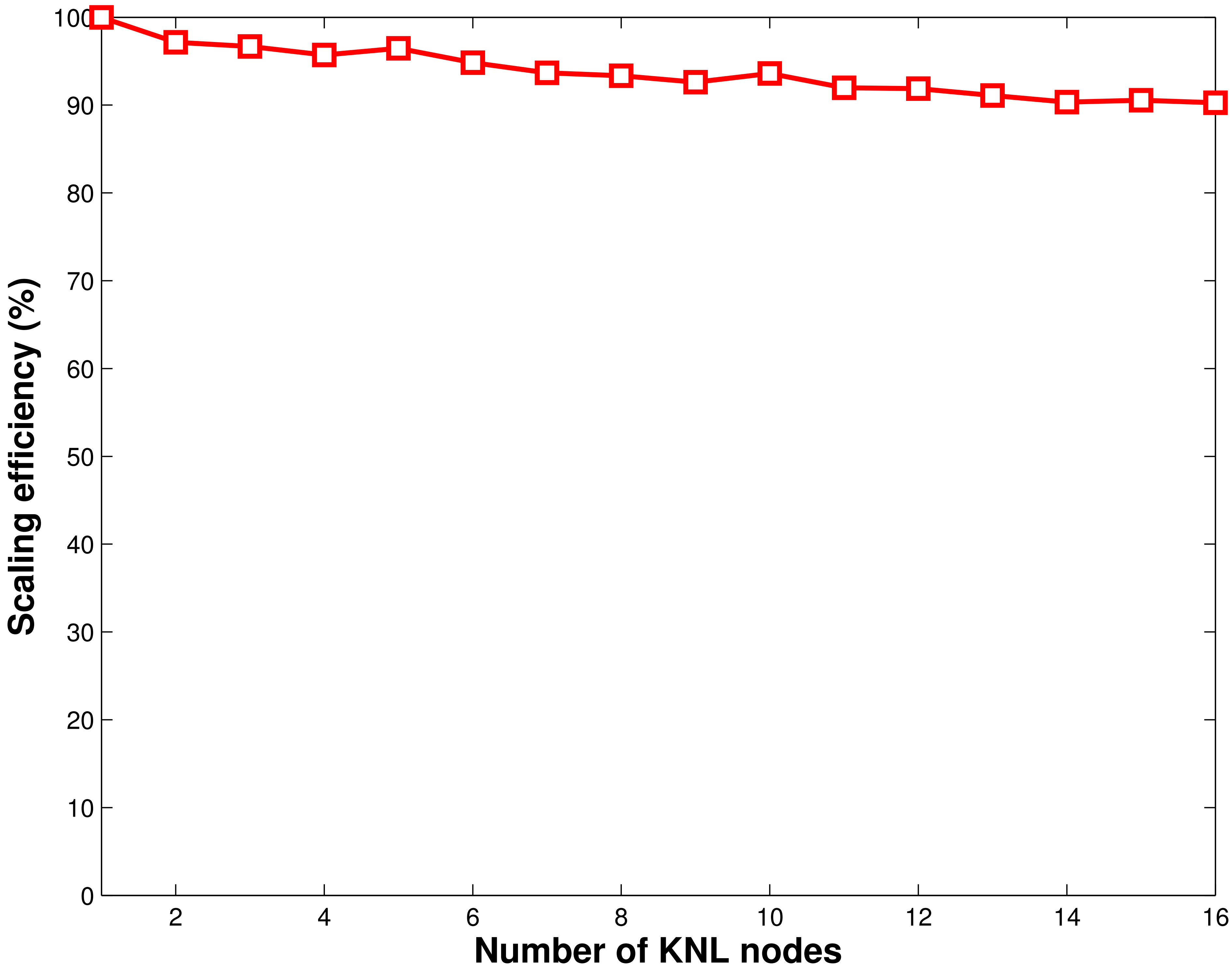
Knights Landing: roofline plot

OCCA version of NUMA



Knights Landing: weak scaling

work in progress



Summary

- Mira:
  - 3.0km baroclinic instability within 4.15 minutes runtime per one day forecast
  - 99.1% strong scaling efficiency on Mira, 1.21 PFlops
- Titan:
  - 90% weak scaling efficiency on 16,384 GPUs
  - GPU: runs up to 15x faster than on one CPU node
- Intel Knights Landing:
  - looks good but still room for improvement

Thank you for your attention!