UNIVERSITÄT PADERBORN
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FPGAs in HPC: Algorithm-Hardware Co-design of a Discontinuous Galerkin Shallow-Water Model for a Dataflow Architecture

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Paderborn Center for Parallel Computing

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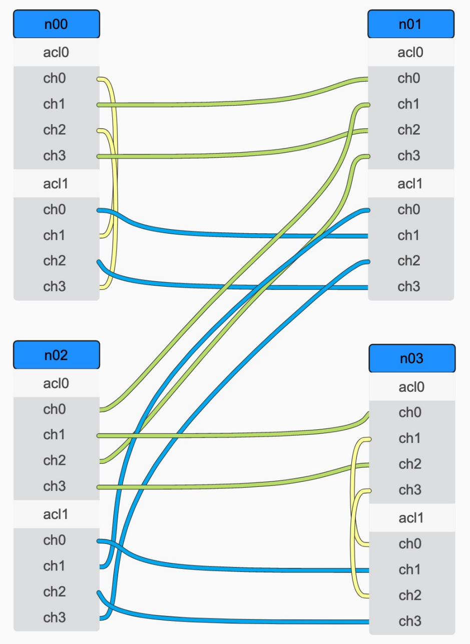
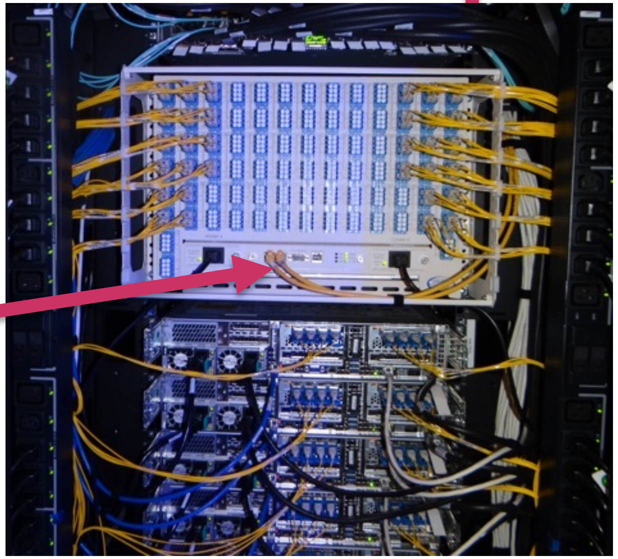
Paderborn Center for Parallel Computing (PC²)

- HPC operations and research
- Noctua System since 2018
  - Cray CS500 Cluster System
  - 256 CPU nodes, 2 x Intel Xeon Skylake Gold 6148, 2 x 20 Cores, 2.4GHz, 192 GB RAM
  - 100 Gbps Intel Omni-Path network
- 16 FPGA nodes
  - 2 x Intel Stratix 10 GX2800 per node (BittWare 520N boards, PCIe 3.0 x8)
    - 4 x 8GB DDR4 channels per board
  - 4 QSFP28 ports per board
  - configurable point-to-point topologies

```
srun -N4 --fpgalink="ring0"
```

- Successor system 2022





FPGA Plattform

- Intel Stratix 10 GX 2800
  - 5760 DSP blocks (1 single precision FMA/cycle each)
  - 11,721 M20K RAM blocks (20Kb each)
  - 933,120 ALMs: control, addresses, all non-FP arithmetic
  - 3,732,480 registers: form pipeline stages

- Bittware 520N card
  - PCIe Gen3 x8 (x16)
  - 4 * 8GB DDR4

- Intel FPGA SDK for OpenCL
- Intel FPGA Add-on for oneAPI Base Toolkit

This work: Discontinuous Galerkin Shallow-Water Model on FPGA

- Shallow-Water Code
  - Discontinuous Galerkin discretization
  - unstructured mesh
  - polynomial orders 0, 1, 2 viable
- Performance challenges
  - not well-suited for vectorization
    - small inner loops, e.g. 3, 6, 9 iterations
  - indirect and irregular memory access
  - strong scaling, simulation of long time scales

- How can FPGAs help?

[T. Kenter, A. Shambhu, S. Faghih-Naini, V. Aizinger. *Algorithm-Hardware Co-design of a Discontinuous Galerkin Shallow-Water Model for a Dataflow Architecture on FPGA.* PASC'21.]

Mapping Code to FPGA Ressources

- Intel Stratix 10 GX 2800
  - 5760 DSP blocks (1 single precision FMA/cycle each)
  - 11,721 M20K RAM blocks (20Kb each)
  - 933,120 ALMs: control, addresses, all non-FP arithmetic
  - 3,732,480 registers: form pipeline stages

FP-arithmetic

unrolling creates small vector units

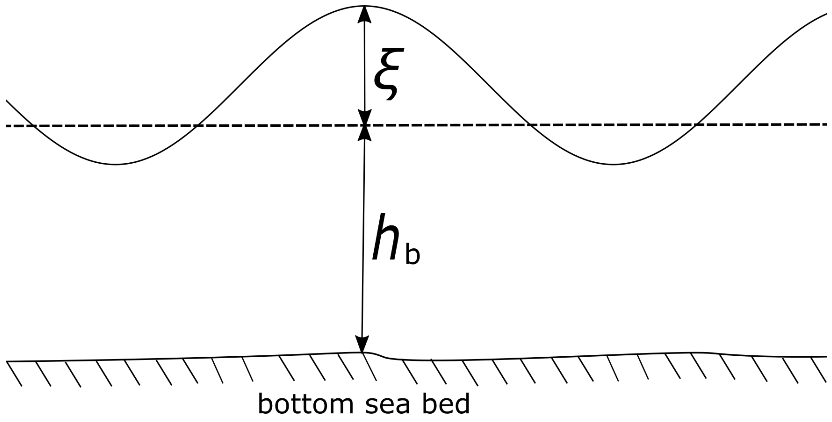
local memory

```
/* Gradient of tidal potential minus athmospheric pressure */
#pragma unroll
for (char i = 0; i < d_space; i++) {
  float temp = G * tip2_l[all_el_info[it].vertex_number[i + 1]] -
               pr2_l[all_el_info[it].vertex_number[i + 1]] -
               G * tip2_l[all_el_info[it].vertex_number[0]] +
               pr2_l[all_el_info[it].vertex_number[0]];
  #pragma unroll
  for (char j = 0; j < d_space; j++)
    tip_pr_grad[j] += all_el_info[it].jacob_phys_to_ref[i][j] * temp;
}
```

Shallow Water DG Code

Shallow Water Equations

- 2D shallow water equations (SWE) (derived from the Navier-Stokes equations)



  - $\partial_t \xi + \nabla \cdot \mathbf{u} = 0$
  - $\partial_t \mathbf{u} + \nabla \cdot \left(\frac{\mathbf{u} \otimes \mathbf{u}}{\mathrm{H}}\right) + \tau_{bf}\mathbf{u} + f_c \mathbf{k} \times \mathbf{u} + \mathrm{gH}\nabla\xi = \mathbf{F}$

with unknowns

ξ : elevation of free water surface, $\mathbf{u} = (U, V)^T$: depth integrated horizontal velocity field

and parameters

h_b: bathymetric depth, $\mathrm{H} = h_b + \xi$: total fluid depth, τ_{bf} : bottom friction coefficient

f_c : Coriolis coefficient, $\mathbf{k}$: unit vertical vector, g : gravitational acceleration

F : forcing term from wind and atmospheric pressure gradient

- Uses Discontinuous Galerkin method on unstructured triangular meshes

$$\int_{\Omega_i} \partial_t \mathbf{c}_\Delta \boldsymbol{\varphi} \, dx + \int_{\partial\Omega_i} \widehat{\mathrm{A}}(\boldsymbol{c}_\Delta, \boldsymbol{c}_\Delta{}^+, \boldsymbol{n}) \, \boldsymbol{\varphi} \, ds - \int_{\Omega_i} \mathrm{A}(\boldsymbol{c}_\Delta) \cdot \nabla\varphi \, dx = \int_{\Omega_i} \boldsymbol{r}(\boldsymbol{c}_\Delta) \, \boldsymbol{\varphi} \, dx$$

Edge kernel | Element kernel

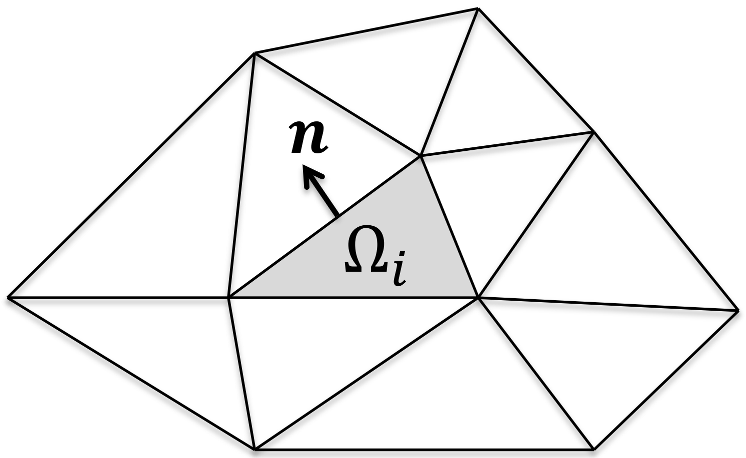
where

$\mathbf{c}_\Delta = (\xi_\Delta, \mathrm{U}_\Delta, \mathrm{V}_\Delta)^T$: the discrete vector of unknowns restricted to Ω_i,

$\mathbf{c}_\Delta{}^+$: the discrete vector of unknowns restricted to the edge-neighbour of Ω_i,

$\boldsymbol{n}$: the exterior unit normal to $\partial\Omega_i$, $\boldsymbol{\varphi}$: test function

$\widehat{\mathrm{A}}$: numerical flux from Riemann solver (Lax-Friedrichs)



UTBEST Overview

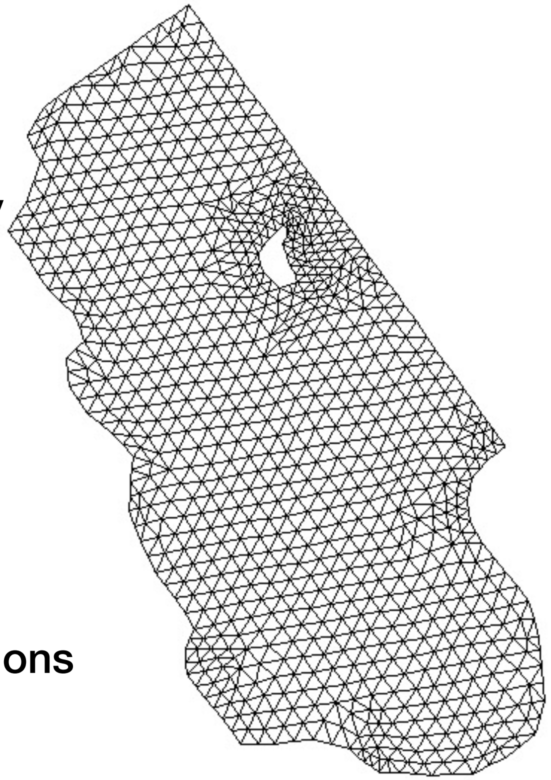
- I/O and grid management: FORTRAN
- DG scheme + computationally intensive parts: C
  - works in single precision
- 3 polynomial DG discretizations
  - piecewise constant (PC) (= cell-centered finite volumes)
  - piecewise linear (PL)
  - piecewise quadratic (PQ)
- Integration kernels
  - elements: 1, 4, 9 quadrature points
  - edges: 1, 2, 3 quadrature points
    - Lax-Friedrichs Riemann solver
- Corresponding time discretization
  - Runge-Kutta orders 1, 2, 3

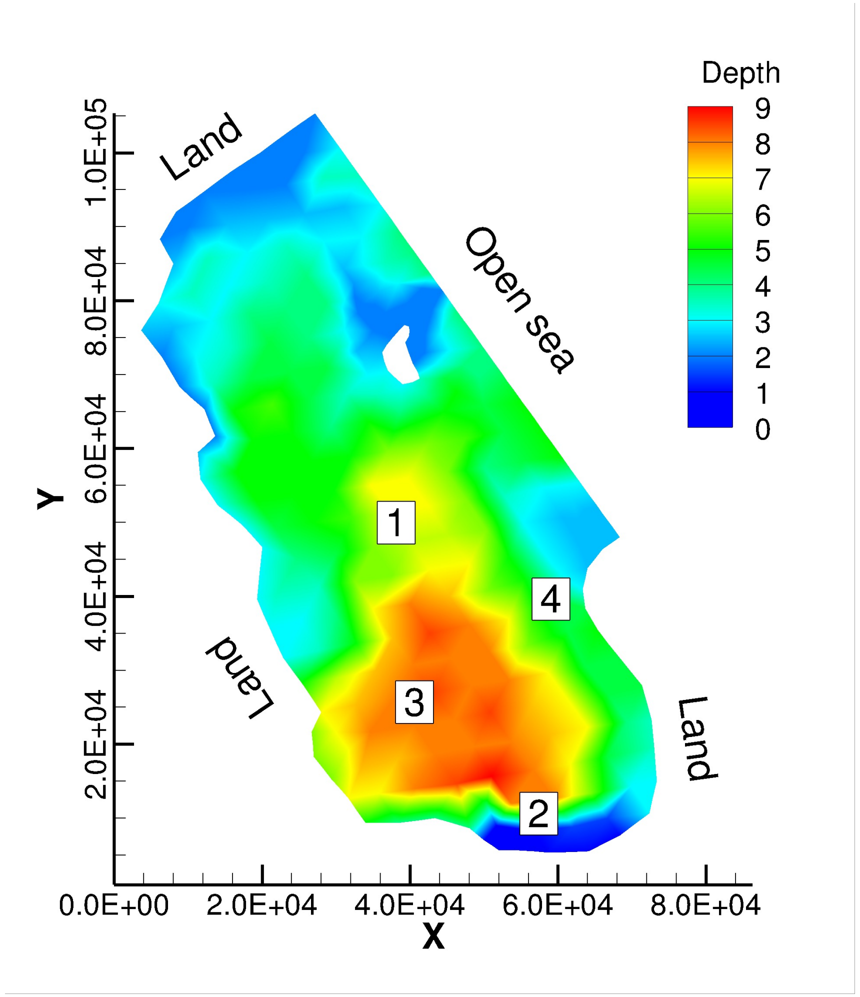
$$\int_{\Omega_i} \partial_t \mathbf{c}_\Delta \boldsymbol{\varphi}\, dx + \underbrace{\int_{\partial\Omega_i} \hat{\mathrm{A}}(\boldsymbol{c}_\Delta, \boldsymbol{c}_\Delta{}^{+}, \boldsymbol{n})\, \boldsymbol{\varphi}\, ds}_{\text{Edge kernel}} - \underbrace{\int_{\Omega_i} \mathrm{A}(\boldsymbol{c}_\Delta) \cdot \nabla\varphi\, dx = \int_{\Omega_i} \boldsymbol{r}(\boldsymbol{c}_\Delta)\, \boldsymbol{\varphi}\, dx}_{\text{Element kernel}}$$

[V. Aizinger and C. Dawson. 2002. Adv. in Water Resources 25, 1]

Benchmark Scenario

- Bahamas (Bight of Abaco)
  - unstructured mesh
    - 1696 elements
  - tidal forcing at open sea boundary
  - benchmark runs
    - simulated 1 day
    - time step 5s
    - 17280 steps
  - outputs
    - elevation snapshots
    - full time series at observation stations





bathymetry + observation stations

UTBEST Structure + Execution

```
while t < t_1 do
  Loop over Runge–Kutta stages:
  for all stages of the Runge–Kutta method do
    Element loop:
    for all element indices e ∈ {1, . . . , E} do
      calculate element integrals
    end for
    Loops over edges of different types:
    for all interior edges do
      calculate interior edge integrals
    end for
    for all land edges do
      calculate land edge integrals
    end for
    for all open sea edges do
      calculate open sea edge integrals
    end for
    calculate c_Δ for the next Runge–Kutta stage
    perform minimum depth control on c_Δ
  end for
  t ← t + Δt
end while
```

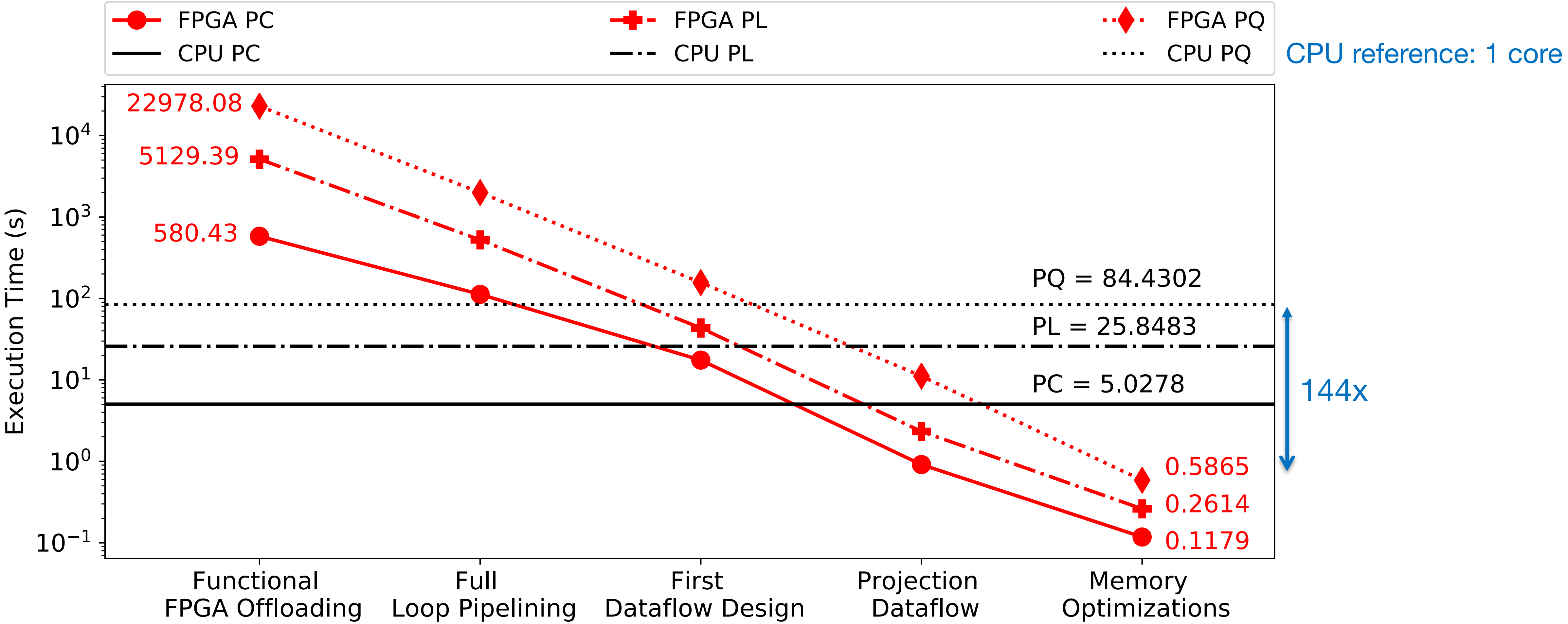
Kernel	Execution time			Perf. [GFLOPs]		
	PC	PL	PQ	PC	PL	PQ
Element	26.9%	38.0%	47.9%	2.27	3.76	4.97
Interior Edge	62.3%	53.2%	44.5%	1.51	2.27	2.97
Land Edge	2.4%	1.8%	1.4%	1.65	2.28	2.85
Sea Edge	2.2%	1.1%	0.6%	0.67	1.30	2.06
Accumulator	2.3%	3.3%	3.9%	2.98	3.92	4.32
Min. Depth	3.8%	2.5%	1.7%	1.40	2.41	3.38
Kernel sum, avg	5.02s	25.8s	84.4s	1.73	2.88	3.98

Profiled on 1 core of Skylake Xeon Gold 6148

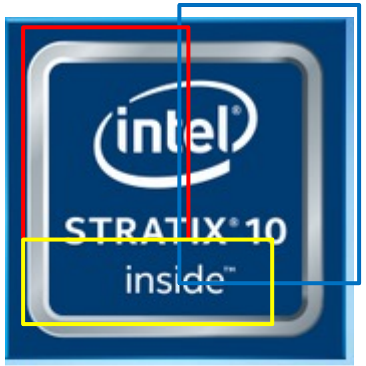
FPGA Design Process

Overview of FPGA Optimization Process

- five main design iterations



FPGA Dataflow Idea 1/2



- C → OpenCL → hardware description
  - create block on FPGA for each kernel
  - e.g. process one element per cycle
    - unrolling
    - provide all data from local buffers
- Stream unknowns and updates through kernels
  - task level parallelism

FPGA Dataflow Idea 2/2

```
while t < t_1 do
    Loop over Runge–Kutta stages:
    for all stages of the Runge–Kutta method do
        Element loop:
        for all element indices e ∈ {1, . . . , E} do
            calculate element integrals
        end for
    end for
    t ← t + Δt
end while
```

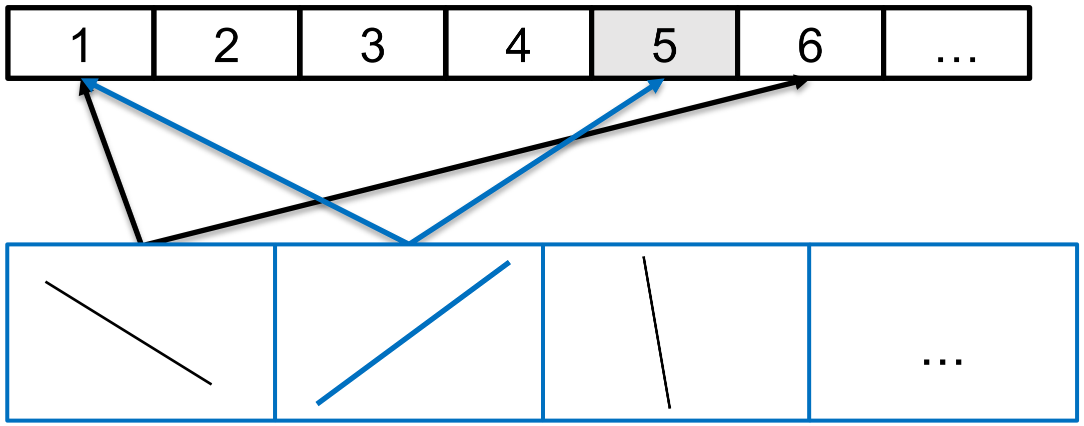
```
while t < t_1 do
    Loop over Runge–Kutta stages:
    for all stages of the Runge–Kutta method do
        perform minimum depth control on c_Δ
    end for
    t ← t + Δt
end while
```

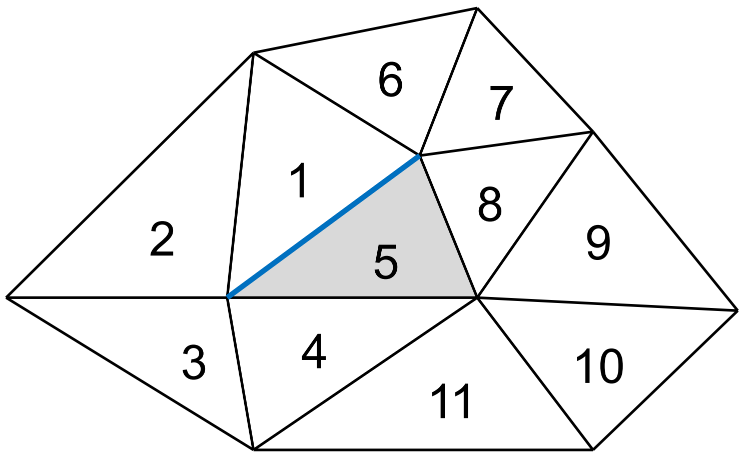
```
while t < t_1 do
    Loop over Runge–Kutta stages:
    for all stages of the Runge–Kutta method do
        calculate c_Δ for the next Runge–Kutta stage
    end for
    t ← t + Δt
end while
```

```
while t < t_1 do
    Loop over Runge–Kutta stages:
    for all stages of the Runge–Kutta method do
        Loops over edges of different types:
        for all interior edges do
            calculate interior edge integrals
        end for
        for all land edges do
            calculate land edge integrals
        end for
        for all open sea edges do
            calculate open sea edge integrals
        end for
    end for
    t ← t + Δt
end while
```

UTBEST Data Layout

- Unknowns $\mathbf{c}_\Delta$ associated to elements
  - 3 * [1, 3, 6] depending on polynomial order





- Further structure by references
  - edges to elements
    - "random" access into element array
  - elements to edges
  - ...
- Geometry, bathymetry

Initial Dataflow around Edge Kernel

- Three phases required

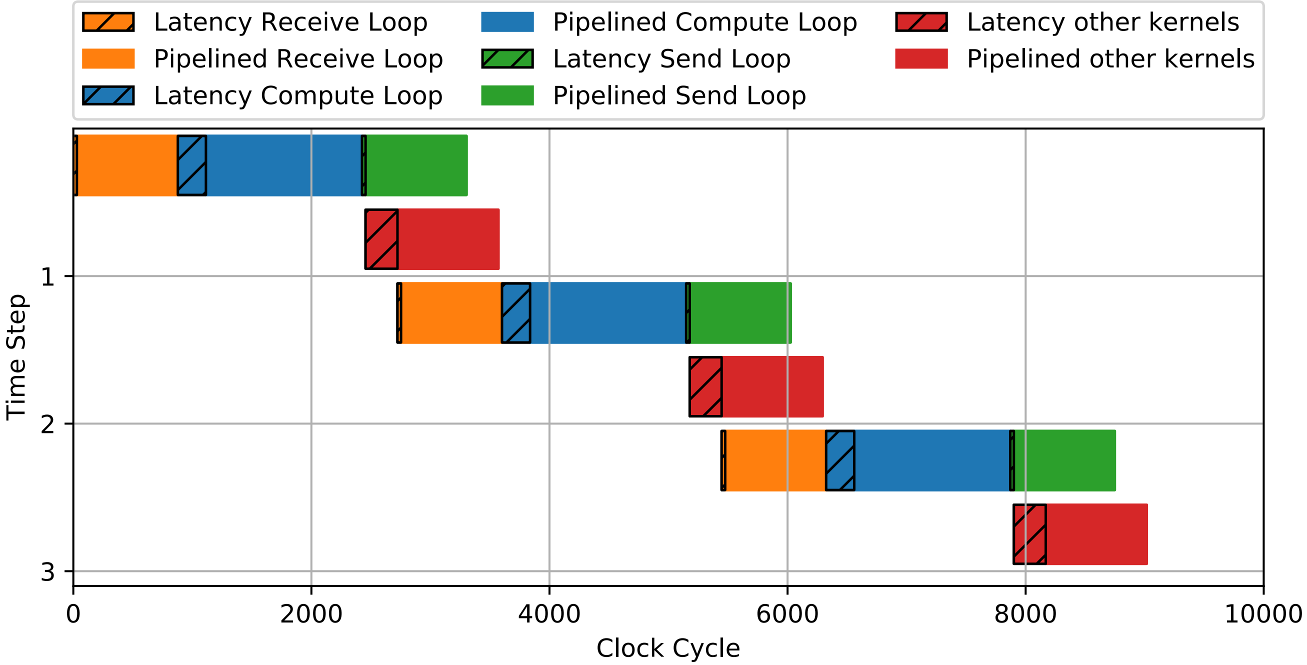
1	2	3	4	5	6	…

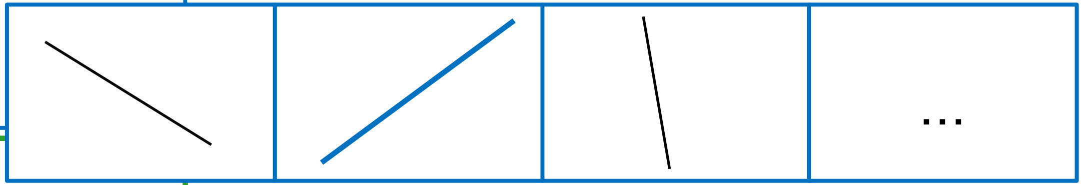
Receive loop:
for all element indices $e \in \{1, \ldots, E\}$ **do**
  receive $\boldsymbol{c}_\Delta$ from minimum depth channel
  initialize element update term $\boldsymbol{r}_{\boldsymbol{flux}}(\boldsymbol{c}_\Delta) \leftarrow \boldsymbol{0}$
end for

Compute loop:
for all edge indices $d \in \{1, \ldots, D\}$ **do**
  flux $\boldsymbol{A}(\boldsymbol{c}_\Delta)$ and solution $\boldsymbol{c}_\Delta$ on local element
  flux $\boldsymbol{A}(\boldsymbol{c}_\Delta^+)$ and solution $\boldsymbol{c}_\Delta^+$ on remote element
  Riemann flux $\hat{\boldsymbol{A}} \leftarrow \boldsymbol{riemann}(\boldsymbol{A}(\boldsymbol{c}_\Delta), \boldsymbol{A}(\boldsymbol{c}_\Delta^+), \boldsymbol{c}_\Delta, \boldsymbol{c}_\Delta^+)$
  update $\boldsymbol{r}_{\boldsymbol{flux}}(\boldsymbol{c}_\Delta) \leftarrow \boldsymbol{r}_{\boldsymbol{flux}}(\boldsymbol{c}_\Delta) - \hat{\boldsymbol{A}}$
  update $\boldsymbol{r}_{\boldsymbol{flux}}(\boldsymbol{c}_\Delta^+) \leftarrow \boldsymbol{r}_{\boldsymbol{flux}}(\boldsymbol{c}_\Delta^+) + \hat{\boldsymbol{A}}$
end for

Send loop:
for all element indices $e \in \{1, \ldots, E\}$ **do**
  send $\boldsymbol{r}_{\boldsymbol{flux}}(\boldsymbol{c}_\Delta)$ to accumulator channel
end for

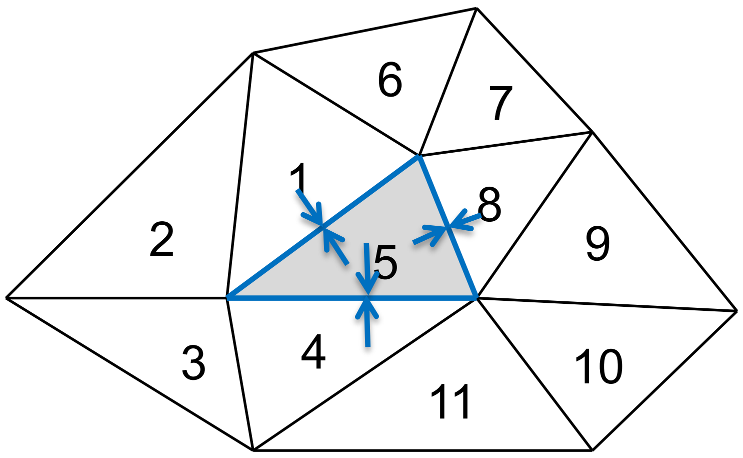
1	2	3	4	5	6	…



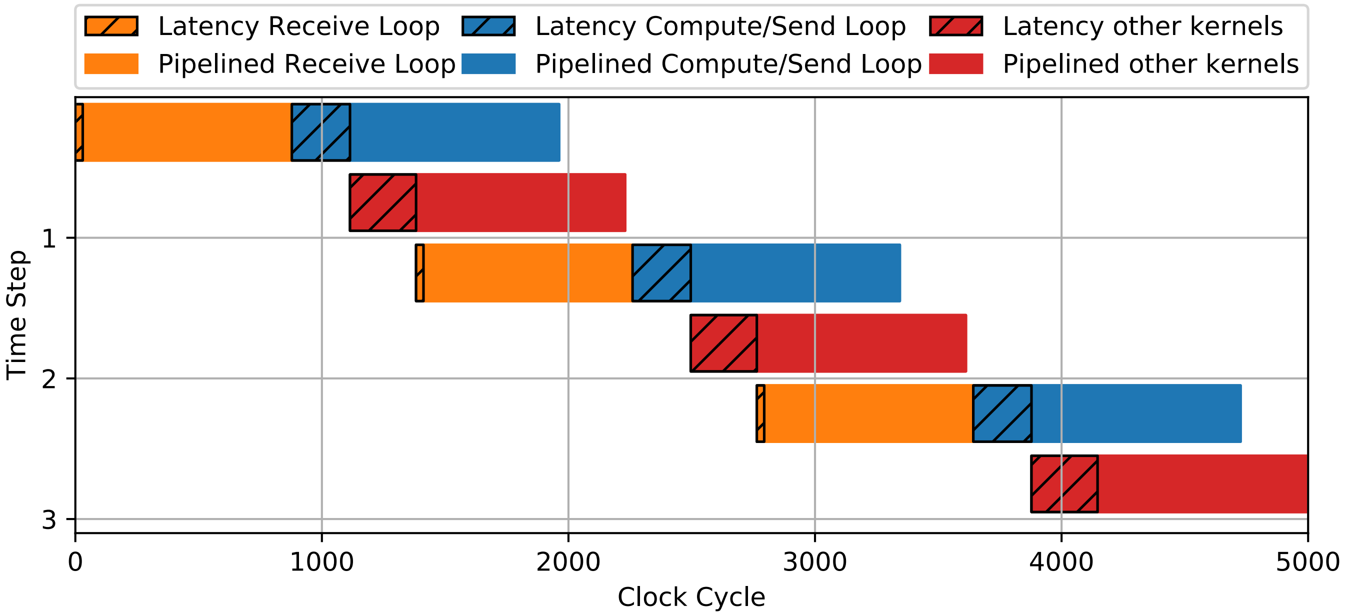


- poor utilization (either edge or element kernel active)
- more edges than elements

- Run edge kernel in order of elements
  - 3 edge integrals per element, each
    - 2 projections to edge
    - 1 Riemann flux
  - perform projections already with element kernel



Receive loop:
for all element $e \in \{1, \ldots, E\}$ **do**
  for all edges belonging to Ω_e **do**
    receive projection $\boldsymbol{p}_\Delta$ from element channel
  end for
end for
Compute and send loop:
for all element $e \in \{1, \ldots, E\}$ **do**
  initialize flux update term $\boldsymbol{r_{flux}}(\boldsymbol{c}_\Delta) \leftarrow 0$
  Loop over three edges per element:
  for all edges belonging to Ω_e **do**
    Riemann flux $\hat{\boldsymbol{A}} \leftarrow riemann(\boldsymbol{A}(\boldsymbol{p}_\Delta), \boldsymbol{A}(\boldsymbol{p}_\Delta^+), \boldsymbol{p}_\Delta, \boldsymbol{p}_\Delta^+)$ (Eq. 10)
    update $\boldsymbol{r_{flux}}(\boldsymbol{c}_\Delta) \leftarrow \boldsymbol{r_{flux}}(\boldsymbol{c}_\Delta) + \hat{\boldsymbol{A}}$
  end for
  send $\boldsymbol{r_{flux}}(\boldsymbol{c}_\Delta)$ to accumulator channel
end for



FPGA Results

Parallelism and Synthesis Results

- Parallel and pipelined operations
  - 1 element integral + projections per cycle
  - 3 edge integrals per cycle
  - accumulation + min. depth 1 element / cycle

- DSPs and logic for arithmetic
- Fit data into block RAMs (8953 available)
  - edge kernel: multiple copies for projection
  - larger mesh requires more space
  - higher order requires more space

FLOPs per element or edge

Order	elements	pro-jection	edges	accum.	min. depth	sum
PC	106	27	$3 \cdot 87$	15	3	412
PL	634	162	$3 \cdot 210$	90	9	1525
PQ	2295	486	$3 \cdot 396$	270	18	4256
PQ CPU	2286	$3/2 \cdot 873$		162	54	3811.5

Synthesis Results

Order	max. elements	Logic Slices	Block RAMs	DSPs	Frequency [MHz]
PC	2048	23%	1923	457	354.17
	4096	24%	2805	457	341.66
	8192	25%	4569	457	312.50
	16384	26%	8083	457	284.38
PL	2048	36%	3037	1194	320.00
	4096	37%	4694	1194	309.37
	8192	39%	7994	1194	285.00
PQ	2048	59%	4924	2773	216.67
	4096	61%	8063	2773	208.33

Performance Model + Example

- Cycles per iteration = #elements + Latency + #external edges
  - e.g. 1696 + 562 + 156 = 2414 cycles for Bahamas benchmark
  - 2414 cycles @ 354.17 MHz = 6.8µs
  - 146715 time steps / s
  - @5s time steps = 8.5 simulated days / s

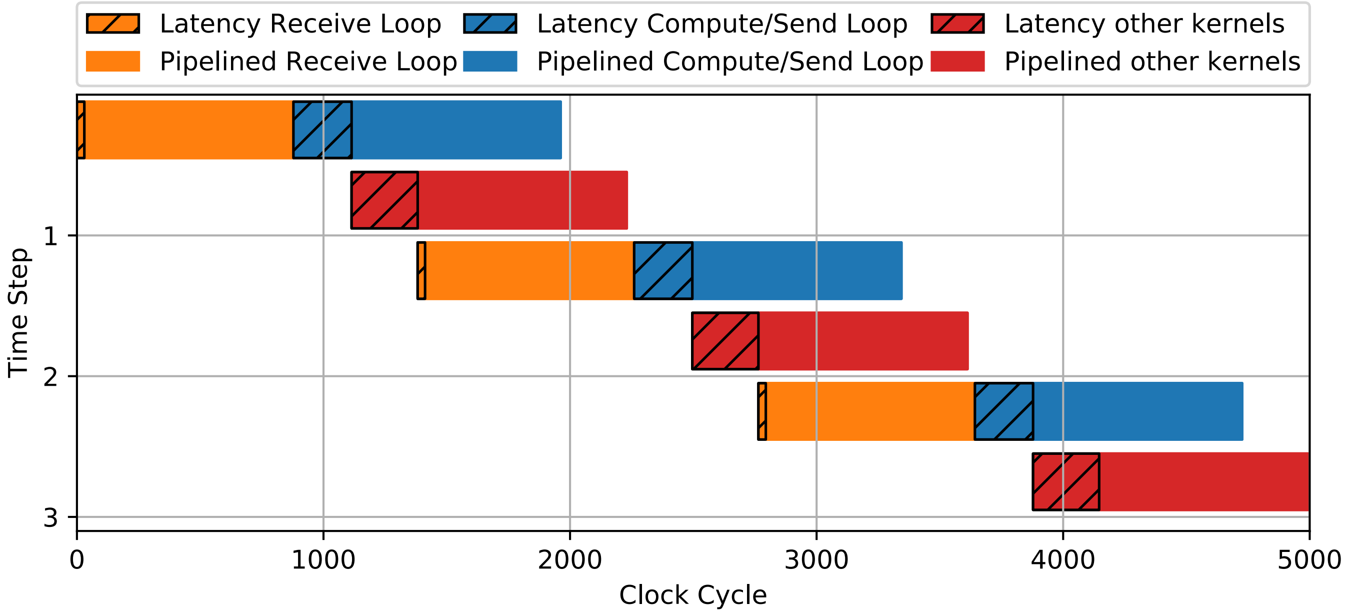


Illustration ~ 1/2 Bahamas, 848 elements

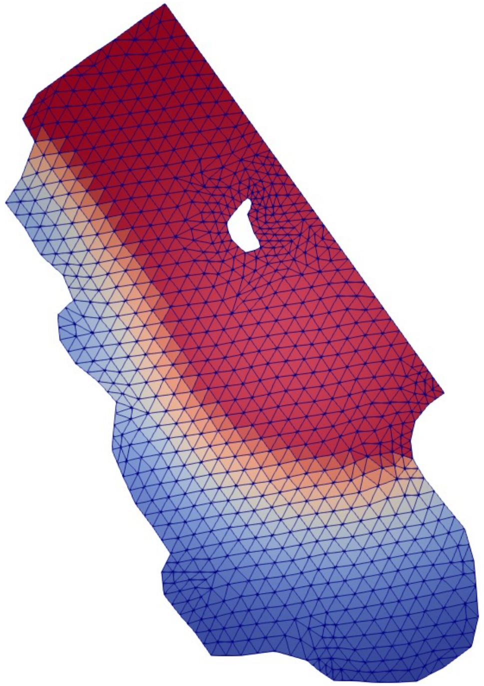
Performance Model vs. Measurements

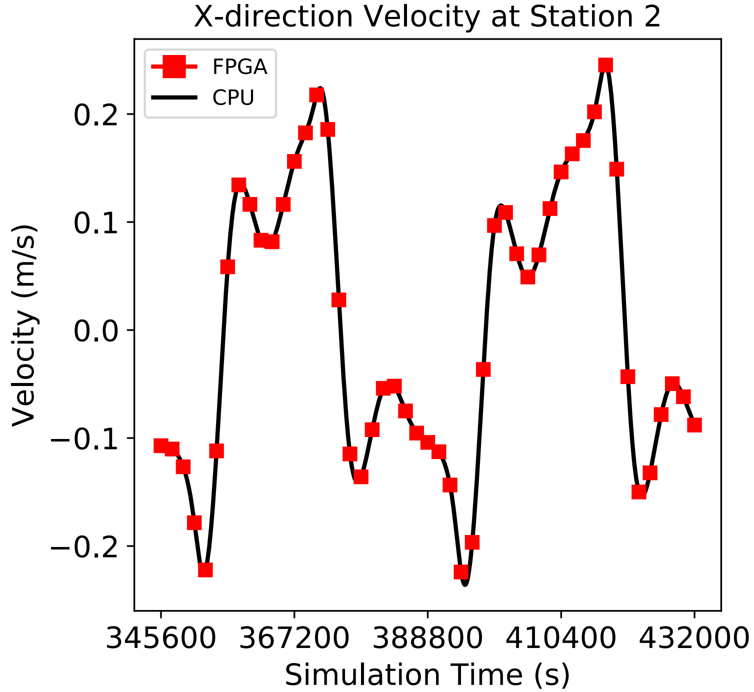
- cycles per iteration = #elements + Latency + #external edges
- occupancy = #elements / cycles per iteration
- FLOPS = Occupancy * peak FLOPS

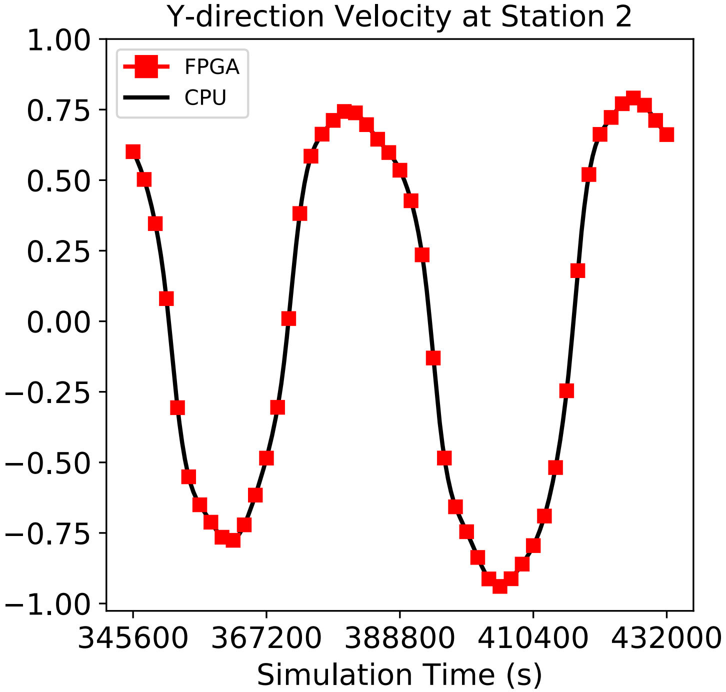
Ord.	E	D_{ext}	L	model *occ.*	model GFLOPs	measured GFLOPs	power [W]
PC	1696	156	562	70.3%	102.5	102.4	74.0
	3392	192	562	81.8%	115.2	114.9	74.5
	6784	312	562	88.6%	114.1	113.9	76.0
	13568	384	562	93.5%	109.5	109.3	77.9
PL	1696	156	569	70.1%	341.9	341.8	76.9
	3392	192	569	81.7%	385.3	384.8	78.5
	6784	312	569	88.5%	384.7	384.1	80.3
PQ	1696	156	592	69.4%	639.9	637.9	77.7
	3392	192	592	81.2%	720.2	717.7	78.9

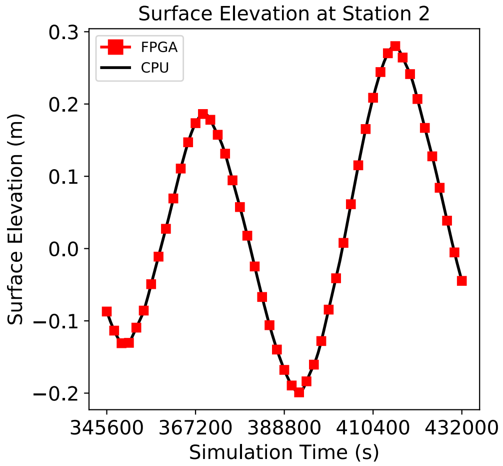
Validation

- Time series and elevation maps
  - only minor numeric differences (due to reordering, rounding)









Ongoing and Future Work

- Scaling
  - multiple pipelines per FPGA for PC, PL
  - multiple FPGAs
  - larger meshes with HBM2 and / or temporal blocking
- Abstractions
  - separation between algorithm and architecture?
- Hybrid execution modes
  - coupling with other models

Summary

- Dataflow architecture on FPGA
  - all kernels in element sequence
  - co-design: projection
- Performance
  - hundreds to thousands operations per cycle
  - up to 720 GFLOPs measured
  - up to 144x speedup over 1 CPU core
  - on small problems