This project has received funding from the European Union's Horizon 2020 Research and Innovation programme under grant agreement No. 801015

EXA2PRO overview

Dr. Lazaros Papadopoulos
ICCS/NTUA

EoCoE EXA2PRO workshop

22 February 2021

EXA2PRO at a Glance

- **Call identifier:** H2020-FETHPC-2017
- **Topic:** FETHPC-02-2017 - Transition to Exascale Computing
- **8 partners from 5 countries**
- **Budget:** 3,475,223 €
- **Duration:** 36 months

- **The project officially ends on 30 July 2021**

EXA2PRO motivation and objectives

exa2pro

Enhancing Programmability and boosting Performance Portability for Exascale Computing Systems

Motivation

Need to support the growth of HPC applications and their transition to exascale.

Currently, **only few applications** are expected to benefit from upcoming exascale computing systems

Main goal

Promote **and lower the barrier of access to exascale computing systems** to scientific community and industry

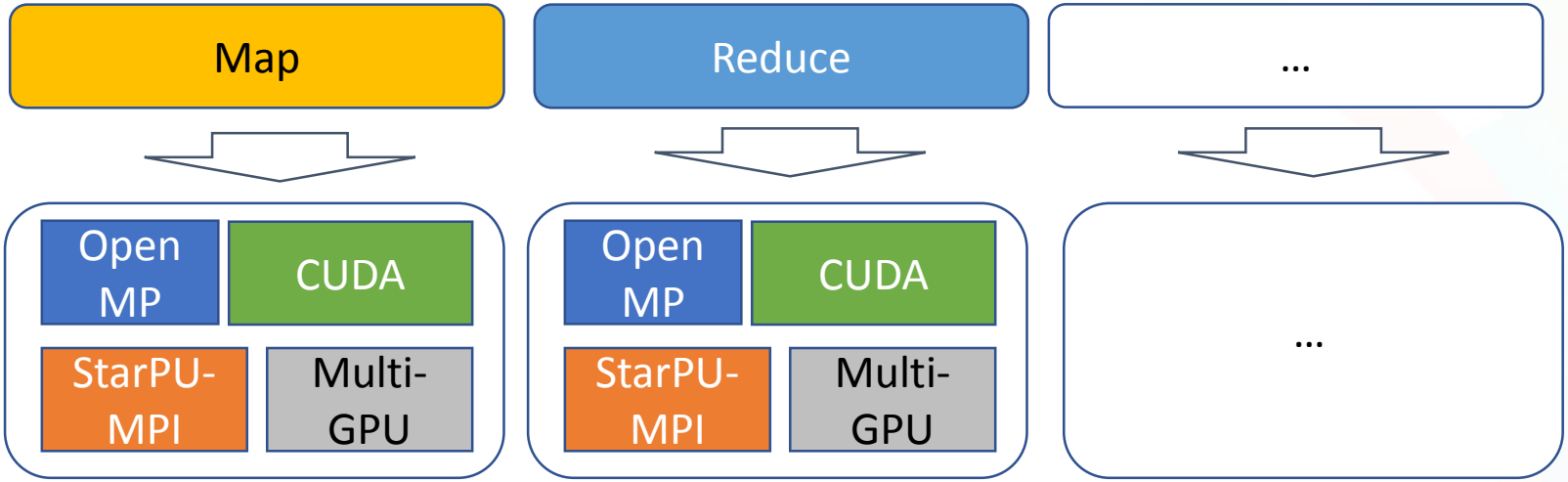
How?

- Exascale systems are expected to be **heterogeneous**
- EXA2PRO improves the programmability of heterogeneous computing systems by **hiding their complexity** from application developers

H2020, Project No. 801015

Main Approach

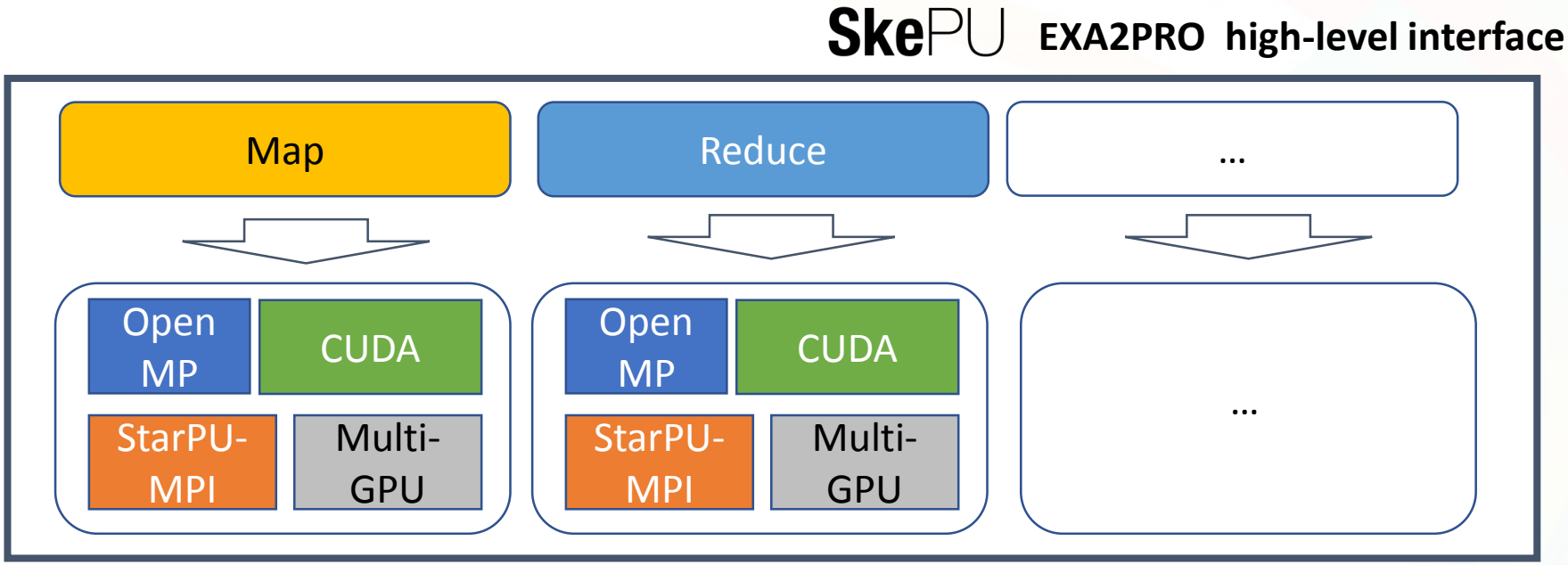
- **Objective 1:** Follow a single-source multiple-backend approach



Patterns of computation implemented for a variety of backends (Skeletons)

Main Approach

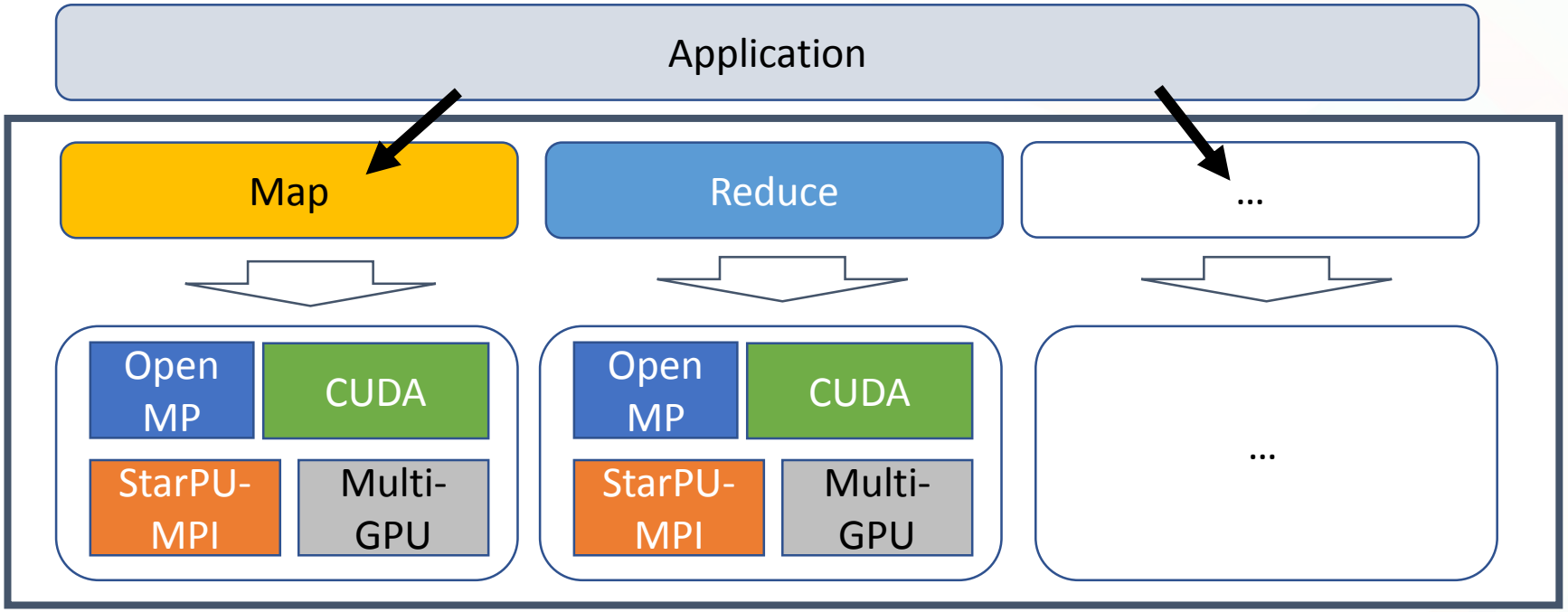
- **Objective 1:** Follow a single-source multiple-backend approach



Patterns of computation implemented for a variety of backends (Skeletons)

Main Approach

- **Objective 1:** Follow a single-source multiple-backend approach



- Patterns of computation implemented for a variety of backends (Skeletons)
- Developers are expected to implement computations of their application through the SkePU EXA2PRO tool

Main Approach

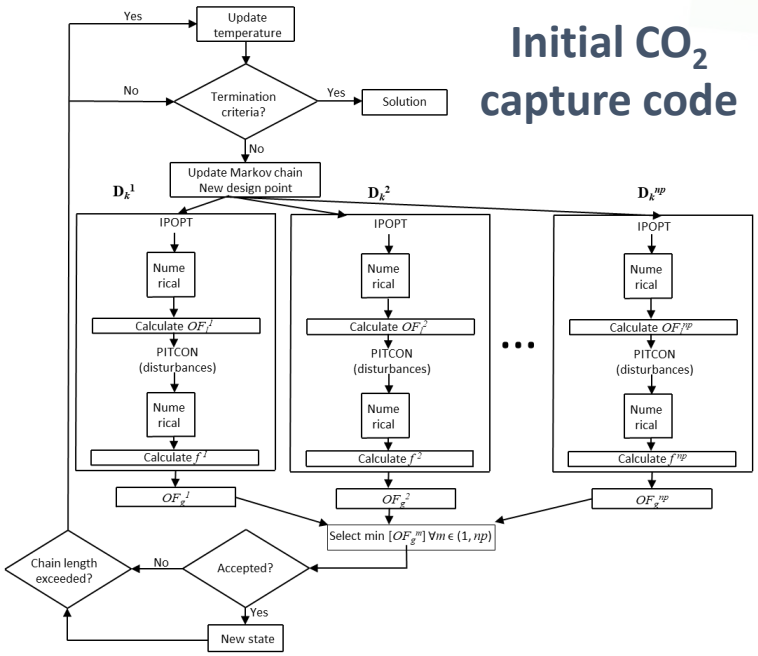
- **Objective 1: Single-source multiple-backend approach**
- **Advantages for application developers:**
  - Experiment with different platforms and accelerators (OpenMP, CUDA, OpenCL-enabled)

Main Approach

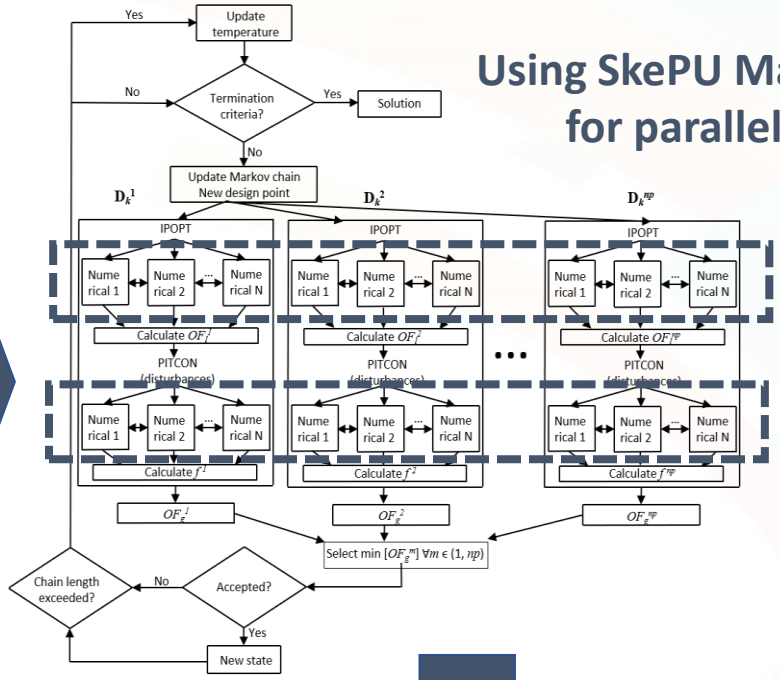
- **Objective 1: Single-source multiple-backend approach**
- **Advantages for application developers:**
  - Experiment with different platforms and accelerators (OpenMP, CUDA, OpenCL-enabled)
  - Can directly use the backend implementations already provided by EXA2PRO SkePU tool. ➔ Productivity

Using EXA2PRO tools to advance the design of material and processes for CO_2 capture

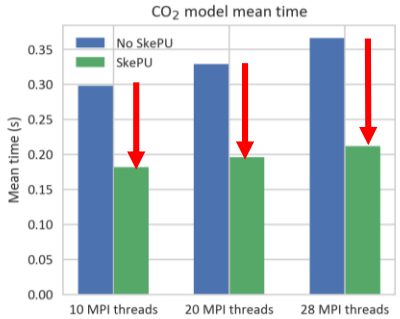
Initial CO_2 capture code

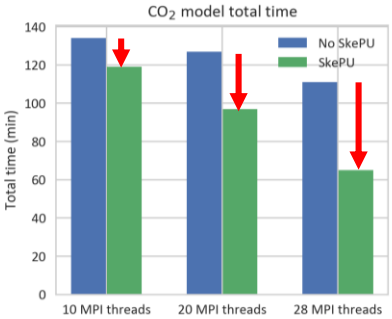


Using SkePU Map skeleton for parallelization



SkePU





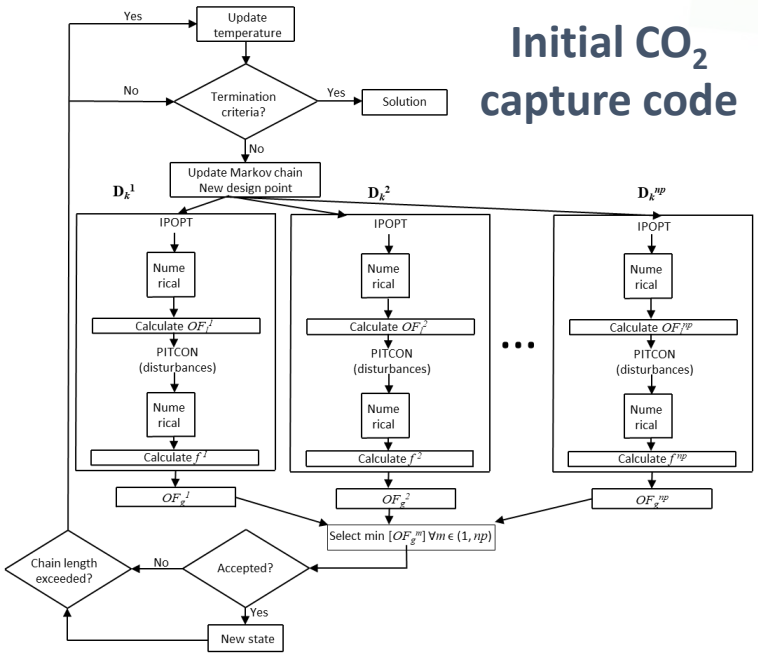
Savings up to 41% of total time by using SkePU version of CO_2 model

N. Vasilas, P. P. Natsiavas, A. Papadopoulos, P. Seferlis, *"Process synthesis and controllability assessment of CO2 capture plants in a parallel environment"*, In Proc. 22nd Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction, 2019.

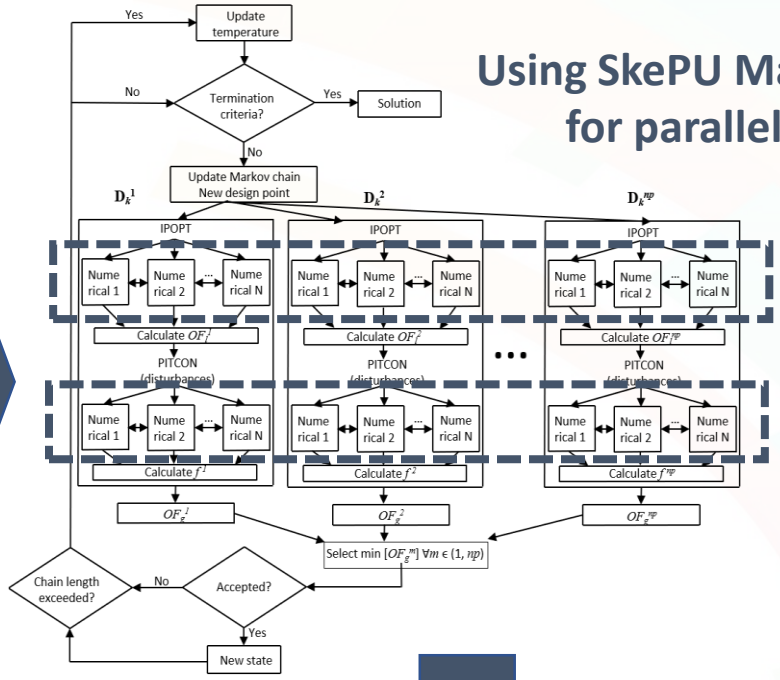
H2020, Project No. 801015

Using EXA2PRO tools to advance the design of material and processes for CO_2 capture

Initial CO_2 capture code



Using SkePU Map skeleton for parallelization



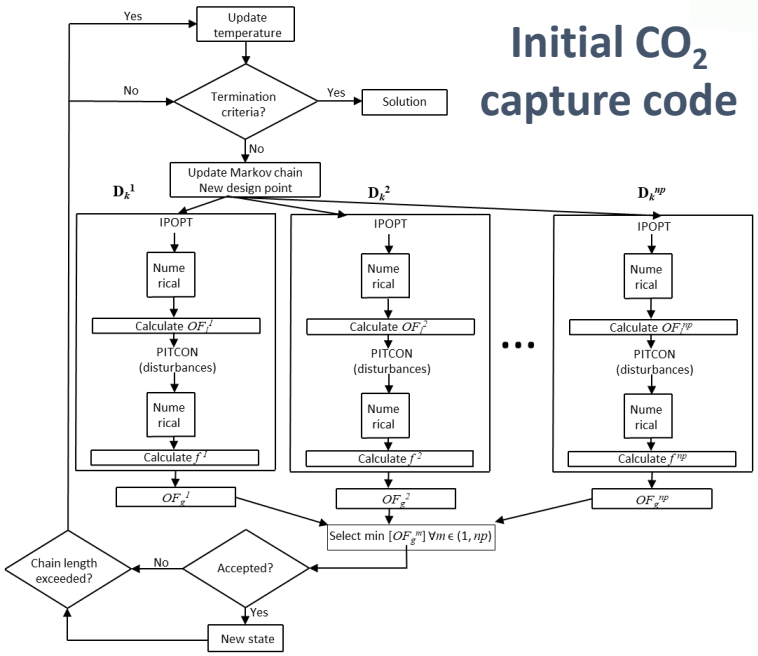
SkePU

Evaluation on GPU
(CUDA & OpenCL)

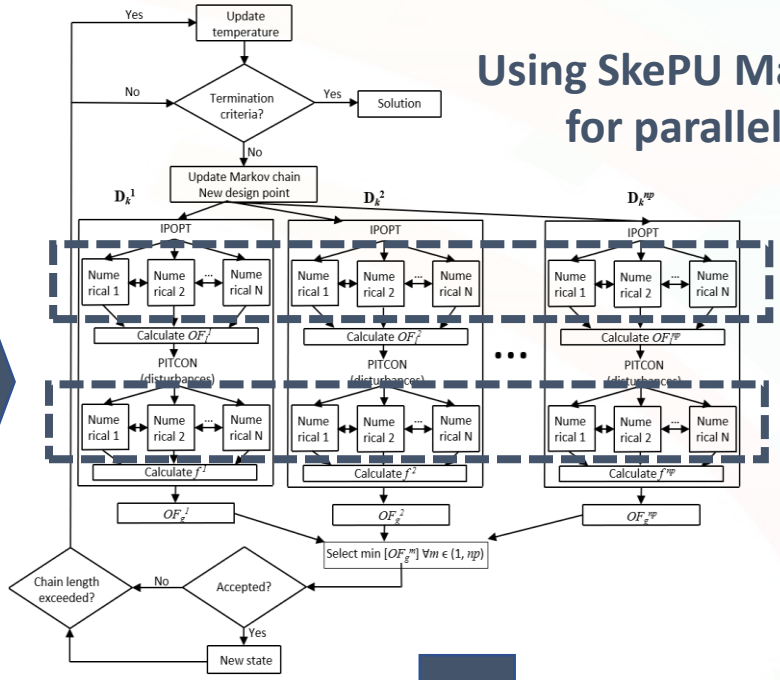
N. Vasilas, P. P. Natsiavas, A. Papadopoulos, P. Seferlis, *"Process synthesis and controllability assessment of CO2 capture plants in a parallel environment"*, In Proc. 22nd Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction, 2019.

H2020, Project No. 801015

Using EXA2PRO tools to advance the design of material and processes for CO_2 capture



Initial CO_2 capture code



Using SkePU Map skeleton for parallelization

SkePU

Accelerators more accessible to developers ➔ transition to systems that use accelerators

Evaluation on GPU
(CUDA & OpenCL)

N. Vasilas, P. P. Natsiavas, A. Papadopoulos, P. Seferlis, *"Process synthesis and controllability assessment of CO2 capture plants in a parallel environment"*, In Proc. 22nd Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction, 2019.

H2020, Project No. 801015

Main Approach

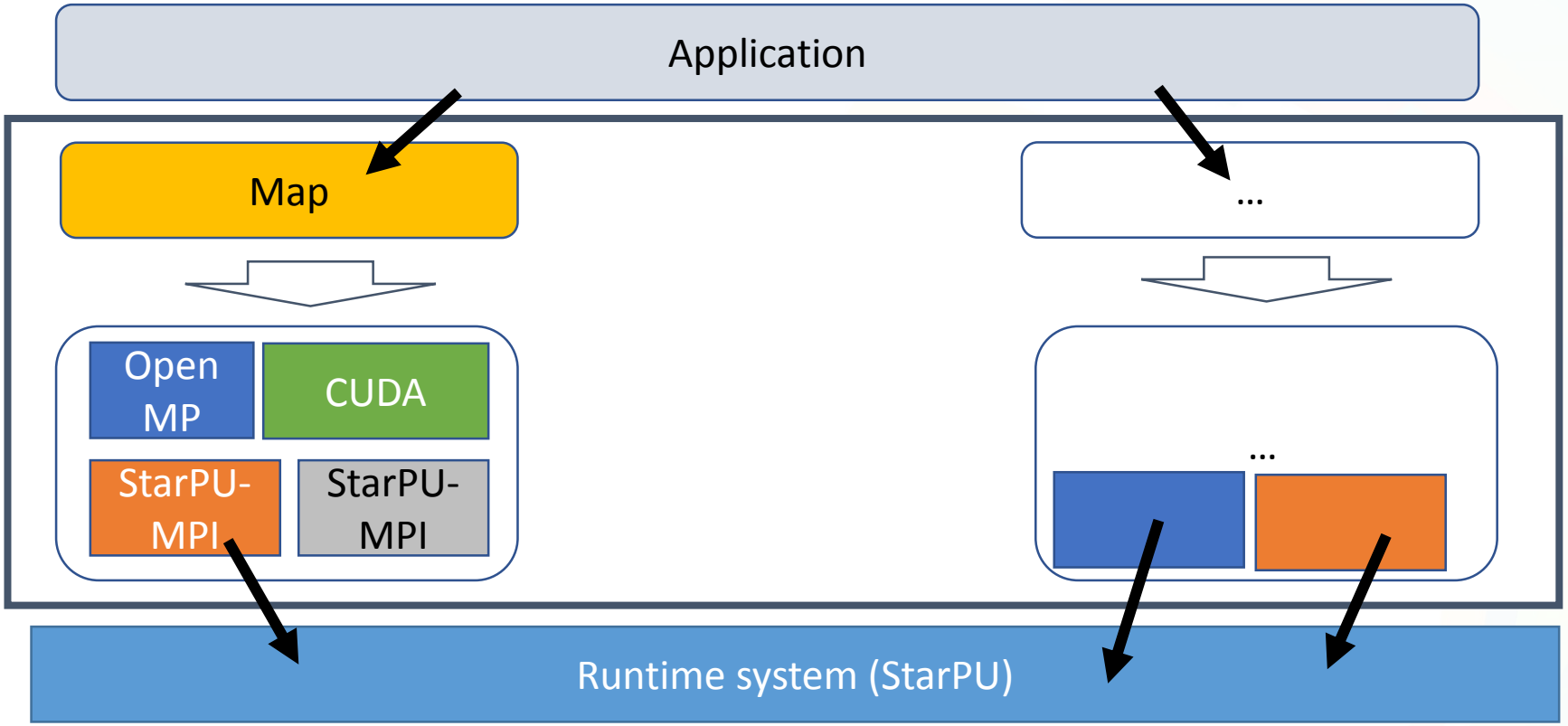
- **Objective 1: Single-source multiple-backend approach**

- **Advantages for application developers:**
  - Experiment with different platforms and accelerators (OpenMP, CUDA, OpenCL-enabled)
  - Can directly use the backend implementations already provided by EXA2PRO SkePU tool. ➔ Productivity

- **The effort to apply the EXA2PRO interface is lower when:**
  - The application is developed in C/C++
  - The computation kernel is well-isolated

Main Approach

- **Objective 1:** Follow a single-source multiple-backend approach

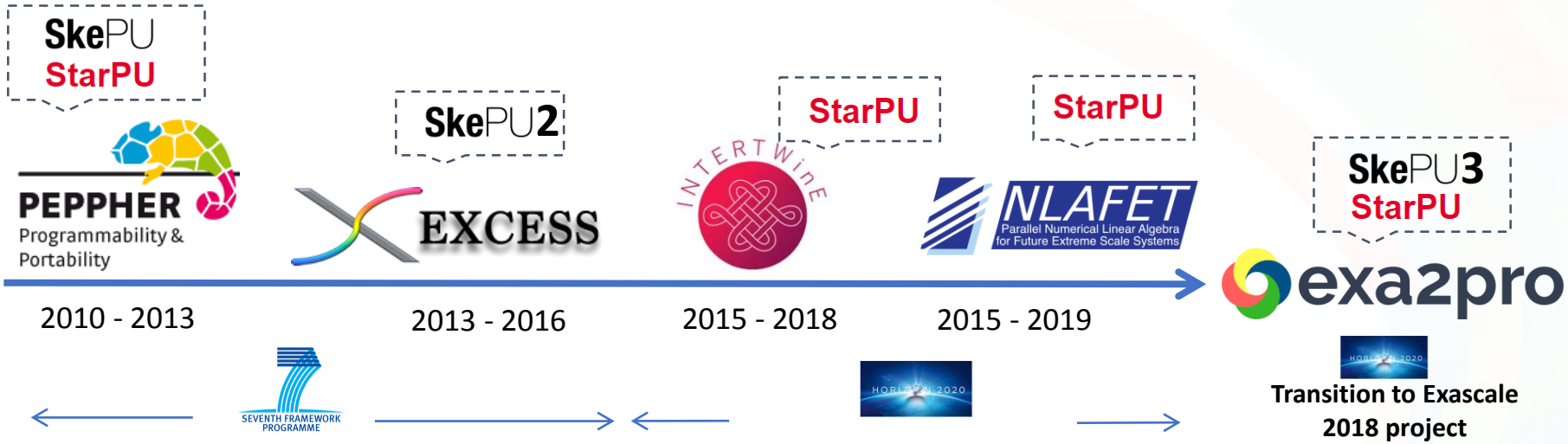


- Elimination of suboptimal or non-applicable backend implementations at design time
- The runtime system selects the most efficient implementation at runtime considering performance and energy as optimization criteria

H2020, Project No. 801015

Main Approach

- **Objective 2:** Co-design approach between tools and applications



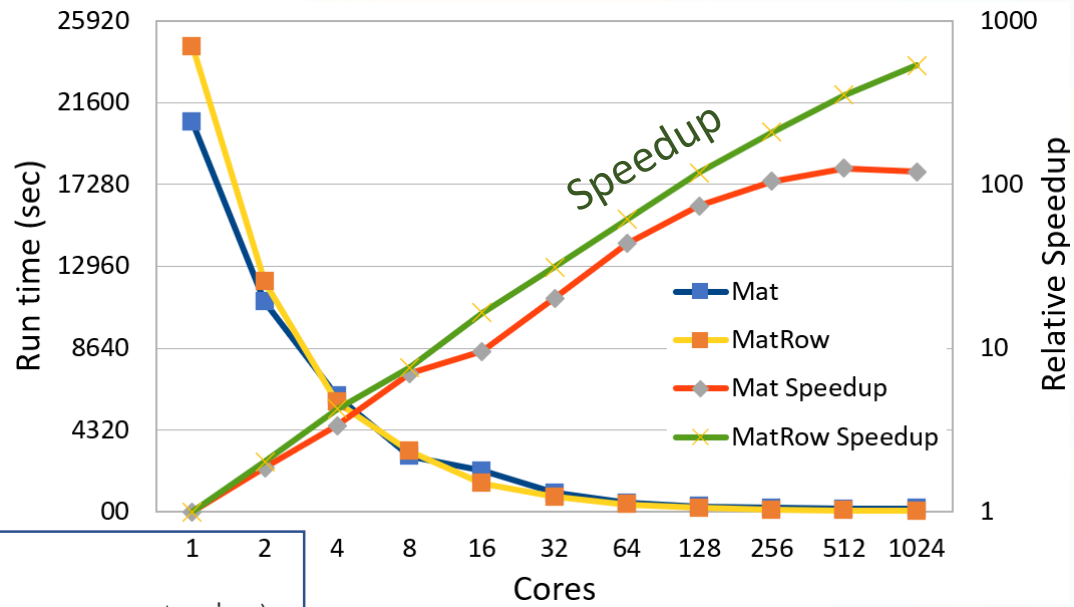
- Tools such as SkePU and StarPU evolve towards exascale computing

Multi-node neural simulations using SkePU

Scaling demonstration across multiple nodes using MatRow SkePU data container (Tetralith cluster: 32 nodes used, 32 cores per node)

Original neural simulation code:

```
for each timestep:
  for each neuron i:
    Get Isyn from adj. Neurons
    … internal dynamics code …
    Compute stateNext[i]
```



SkePU-ported neural simulation code:

```
Function advanceState(i,stateNow,conn_matrix):
  Get Isyn from adj. Neurons
  … internal dynamics code …
  Return stateNext for neuron i

Kernel = Map(get_stateNext)
for each timestep:
  stateNext = Kernel(stateNow,conn_matrix)
```

SkePU
https://skepu.github.io/

Presented in **SCOPES 2020** (25-26 May 2020)
https://scopesconf.org/scopes-20/

S. Panagiotou, A. Ernstsson, J. Ahlqvist, L. Papadopoulos, C. Kessler and D. Soudris, "Portable exploitation of parallel and heterogeneous HPC architectures in neural simulation using SkePU", SCOPES 2020.

H2020, Project No. 801015

Main Approach

- **Objective 3:** Evaluation the data-flow programming model
  - Used to program the FPGA-based MAXELER data-flow engines (DFEs)

MAXELER Technologies

Results: Metalwalls (Simulator for supercapacitors)

Initial results of porting Metalwalls on DFE:

4x performance gain

10x lower energy consumption

50% higher performance/watt than P100 GPU

H2020, Project No. 801015

Results: Metalwalls (Simulator for supercapacitors)

Initial results of porting Metalwalls on DFE:

4x performance gain

10x lower energy consumption

50% higher performance/watt than P100 GPU

Development time: 8 – 12 months ➔ Tools to improve productivity for accessing accelerators

H2020, Project No. 801015

Results: Metalwalls (Simulator for supercapacitors)

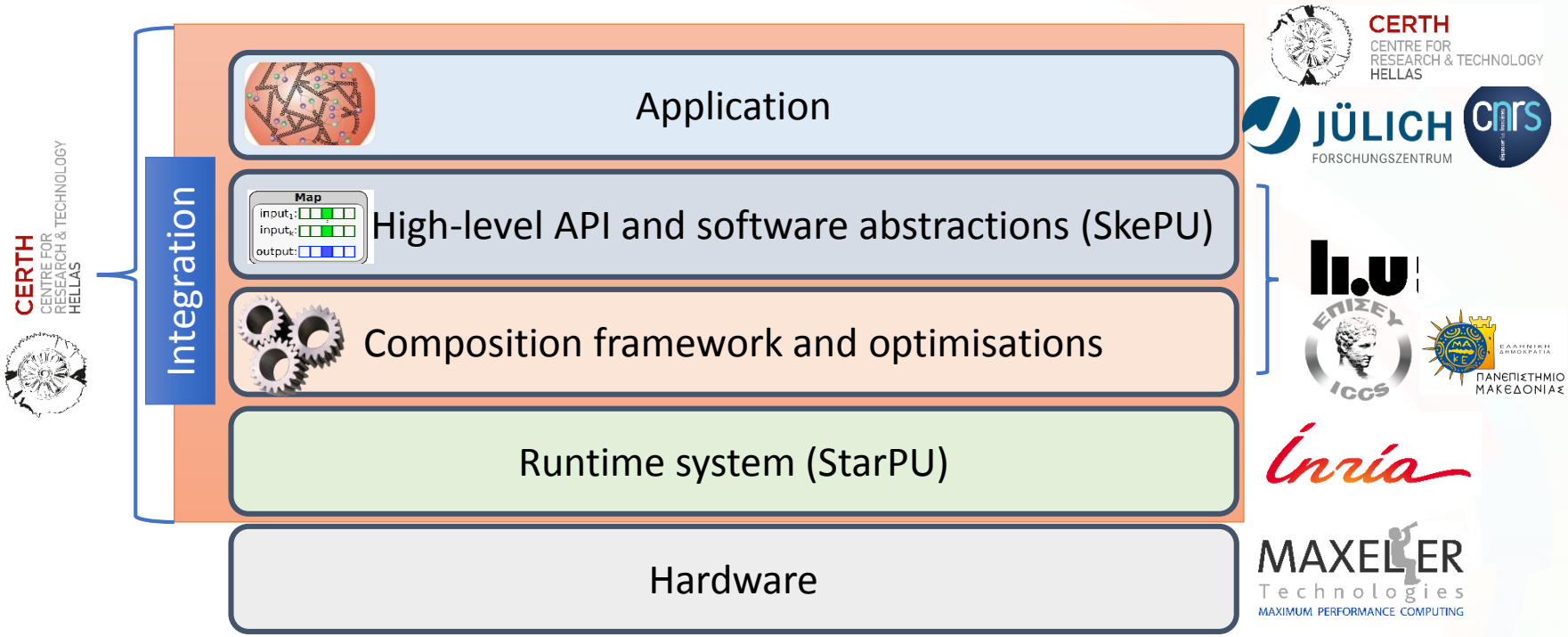
Initial results of porting Metalwalls on DFE:
4x performance gain
10x lower energy consumption
50% higher performance/watt than P100 GPU

Development time: 8 – 12 months ➔ Tools to improve productivity for accessing accelerators

Next step: Use Metalwalls with StarPU for multi-DFE experiments

H2020, Project No. 801015

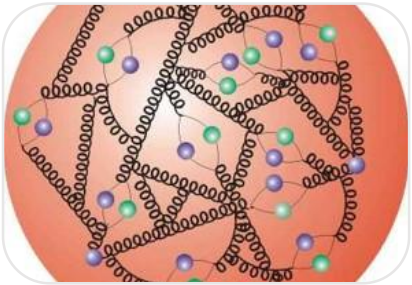
The EXA2PRO stack



H2020, Project No. 801015

EXA2PRO applications

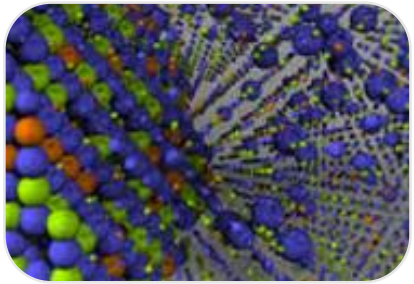
High energy physics



LQCD

- JUELICH
- FORTRAN/C++

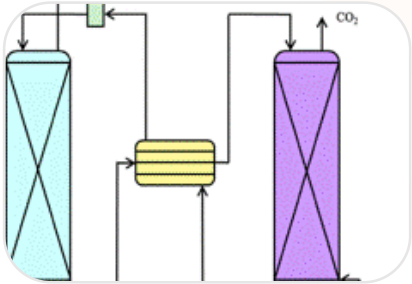
Materials science



KKRNano

- JUELICH
- FORTRAN

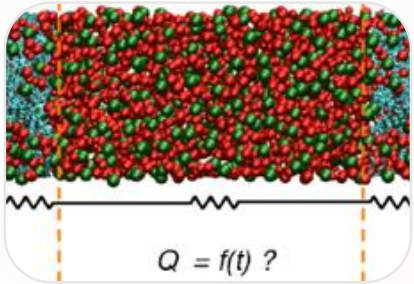
Materials and Processes



Materials and processes for CO_2 Capture

- CERTH
- FORTRAN

Energy



MetalWalls (Supercapacitors simulator)

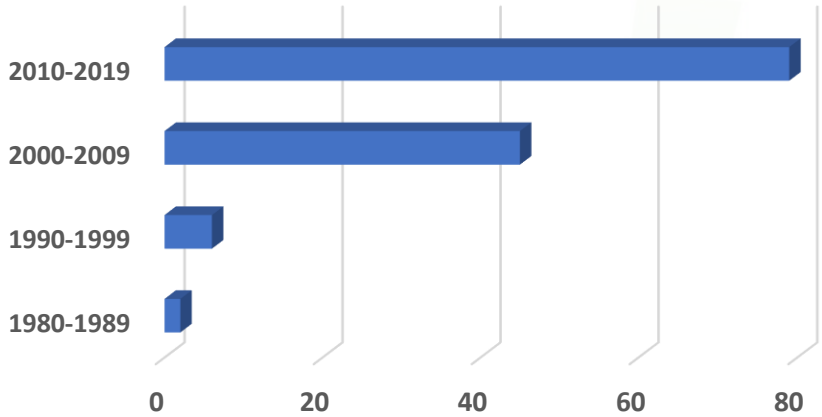
- CNRS
- C++

Applications deployed in pre-exascale systems targeting exascale systems

Applications deployed in HPC clusters
➔ Target large-scale systems

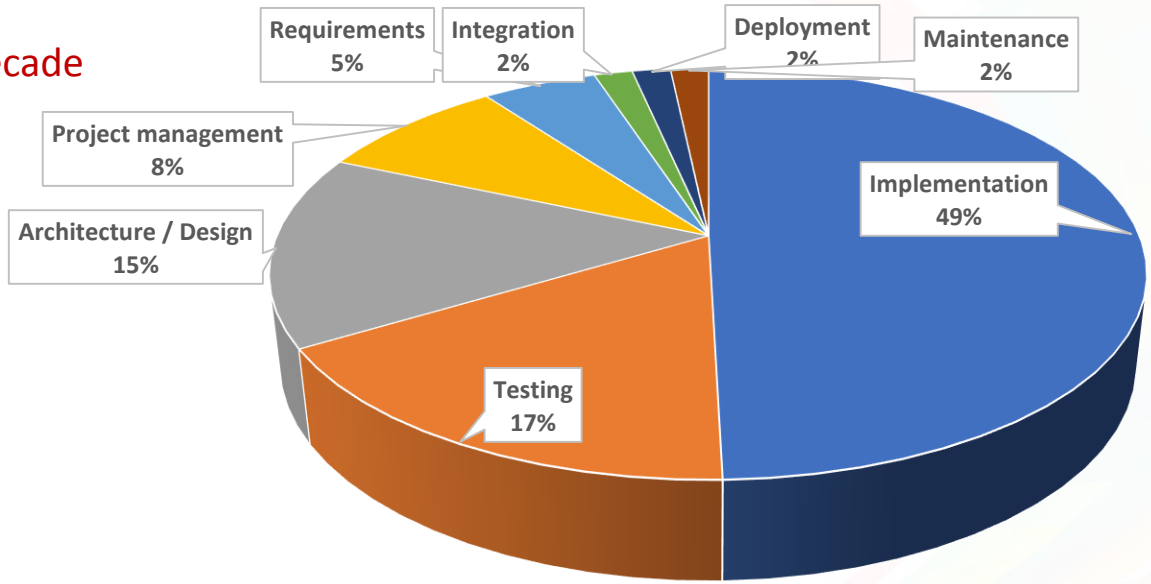
H2020, Project No. 801015

Other aspects: Software engineering practices in HPC



Number of studies per decade

*Studies in the **HPC domain** that employ **Software Engineering** practices*



Number of studies per development phase

In the EXA2PRO, we developed a tool for improving the maintainability of HPC applications, supporting C/C++ and FORTRAN

https://exa2pro.eu/#developers

H2020, Project No. 801015

Conclusions and lessons-learned

- Tool support for accessing accelerators can significantly improve the productivity of application developers
- Interaction between tool developers and application providers was very constructive
  - Contributed to the maturity of the tools and to the application performance improvement
- Data-flow programming is difficult but initial results are very promising

H2020, Project No. 801015

exa2pro

www.exa2pro.eu

Thank You!

lpapadop@microlab.ntua.gr

@exa2pro_h2020

This project has received funding from the European Union's Horizon 2020 Research and Innovation programme under grant agreement No. 801015

Partners
ICCS, LIU, CERTH, INRIA, JUELICH, MAXELER, CNRS, UoM