SPH-EXA: The code for ExaPHOEBOS - Hydrodynamics and gravity at Exa-scale

PIs: Florina Ciorba, Lucio Mayer, Ruben Cabezon

Sebastian Keller, May 24th 2022

The PASC SPH-EXA project

- **SPH and N-body solver for Exascale, flagship application: ExaPHOEBOS, the first 1 trillion particle simulation with SPH and gravity**

- **Synthesis of 3 SPH production codes, stripped down to the essentials**

- **Designed from scratch for Exascale in C++17 with test-driven development and continuous integration.**

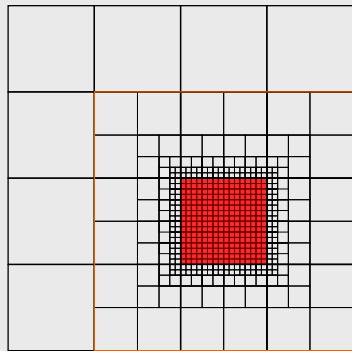- **Developed at University of Basel, Zürich and CSCS**
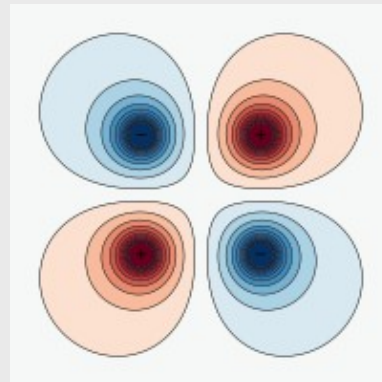
SPHYNX

ChaNGa

NEXTFLOW

SPH EXA

SPH-EXA modules

Cornerstone

octree and domain framework
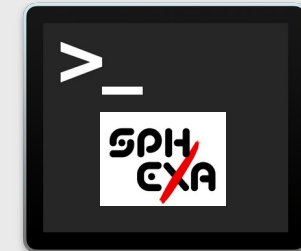
Ryoanji

N-body solver

SPHYNX

ChaNGa

NEXTFLOW

SPH

Hydro solver

SPH-EXA frontend

I/O and test case setup

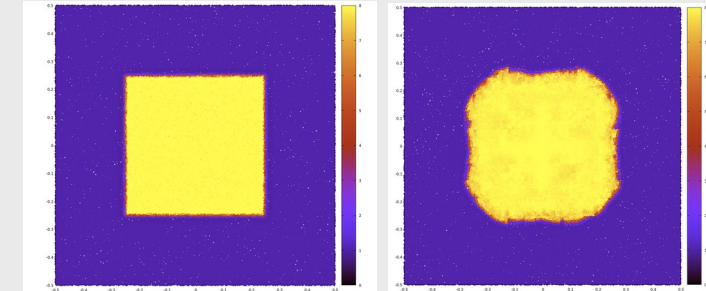# SPH-EXA frontend: test case validation effort

SPH-EXA frontend

Input options:
- Parallel HDF5 I/O from file
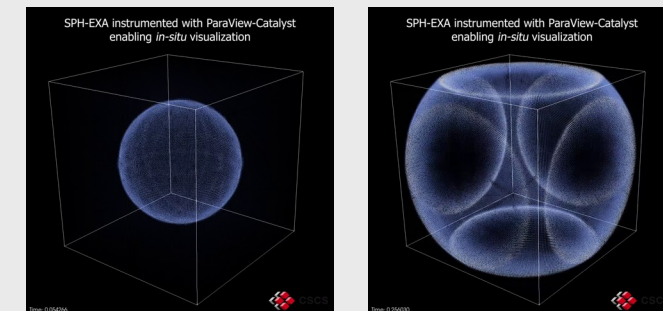- Named test cases

Tests in progress:

- **Kelvin-Helmholtz**
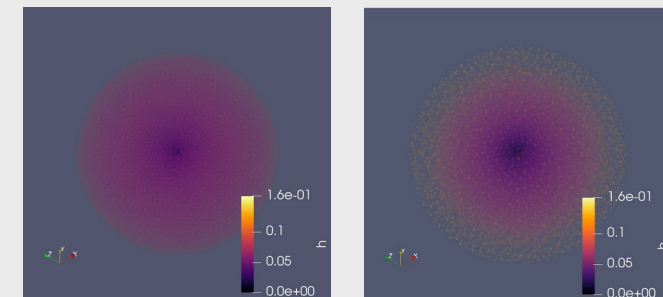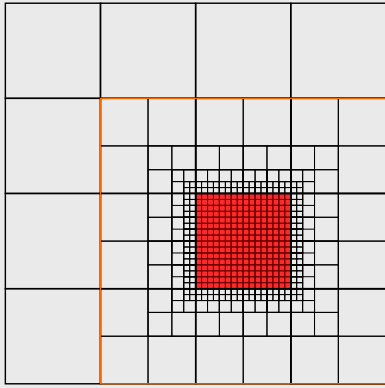- **Raleigh-Taylor**
- **Wind-blob**

Isobaric cube

Sedov blast

Evrard collapse

Cornerstone Octree

Cornerstone octree
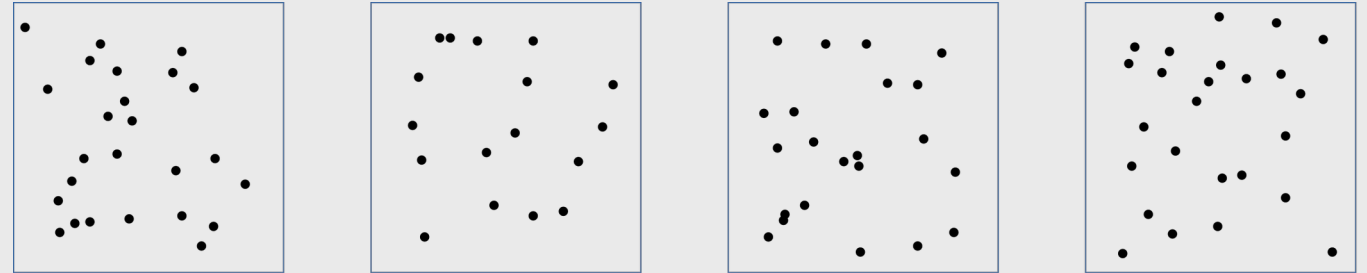
Highly scalable octree and
domain decomposition framework

- **Full GPU acceleration**
- **Leverages collision detection algorithms
  from 3D graphics**
- **Neighbor searching**
- **Halo discovery and exchange**
- **Spatial decomposition along space filling curves**

```
domain.sync(x, y, z, m, q, … );
```
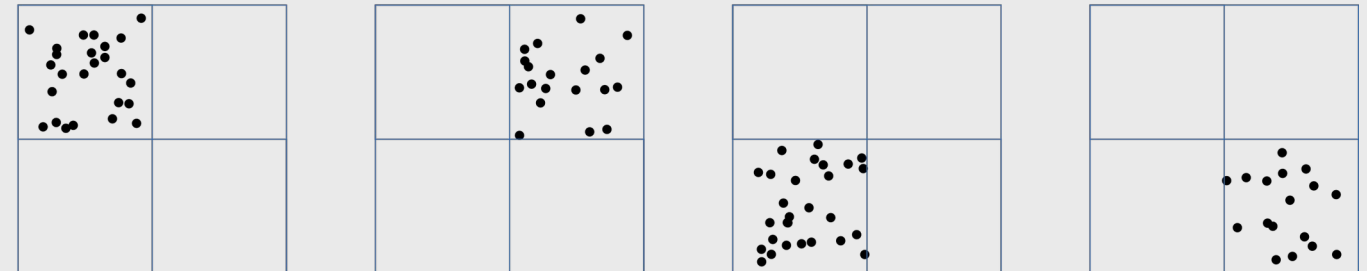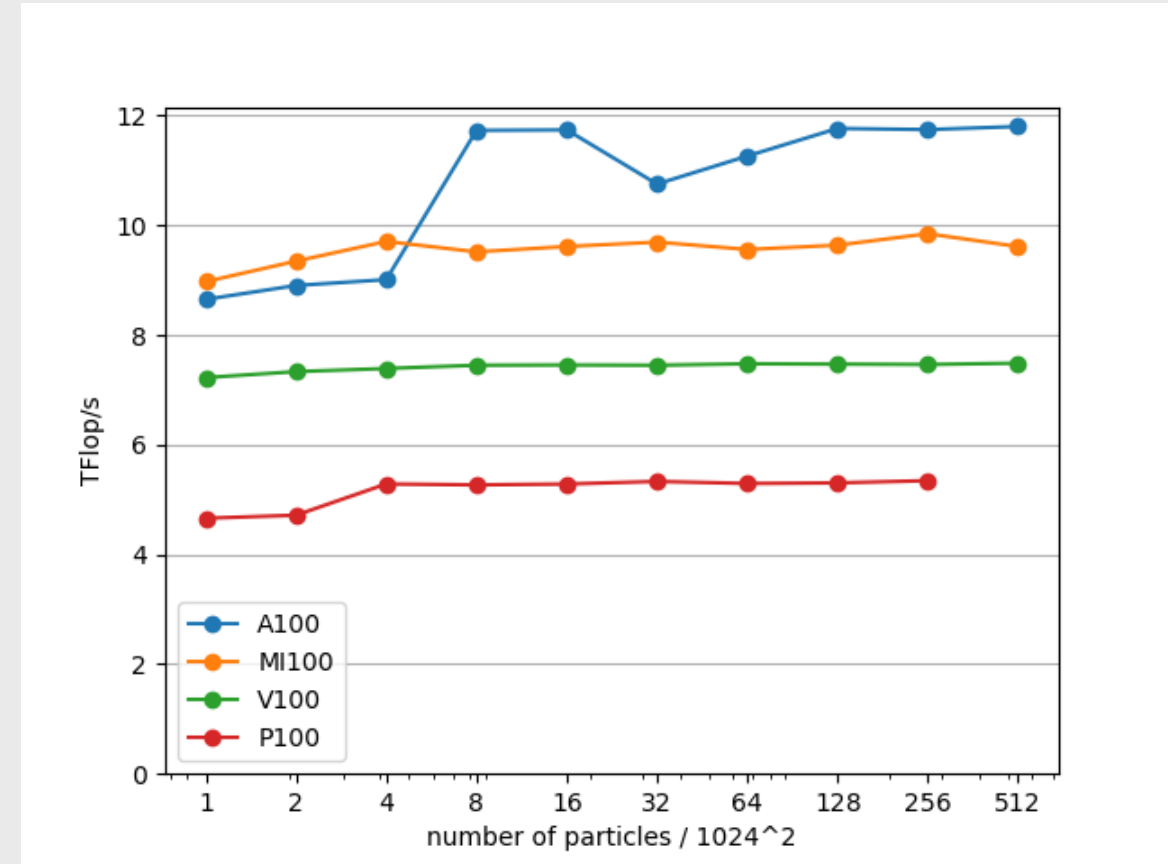
Ryoanji N-body solver
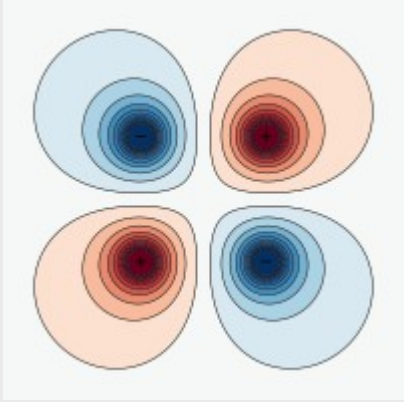
Ryoanji N-body

Gravity and electrostatics solver on the GPU

- **Octree format: Cornerstone**
- **EXA-FMM multipole kernels of arbitrary order**
- **Breadth-first traversal on GPU inspired by Bonsai**
- **Warp (32 threads, NVIDIA) and wave (64 threads, AMD) aware**
- **70-80 % peak flop on A100**

SPH performance, hydrodynamics only

Sedov blast wave on full Piz Daint

- **Testing absolute performance, domain decomposition and halo-exchange**

- **Can scale to full machine**

- **Can scale to ~1 trillion particles (Example here: 0.314 trillion particles full double precision)**

SPH-EXA, Sedov 64e6 particles per node, weak scaling
max particles: 314.4 billion
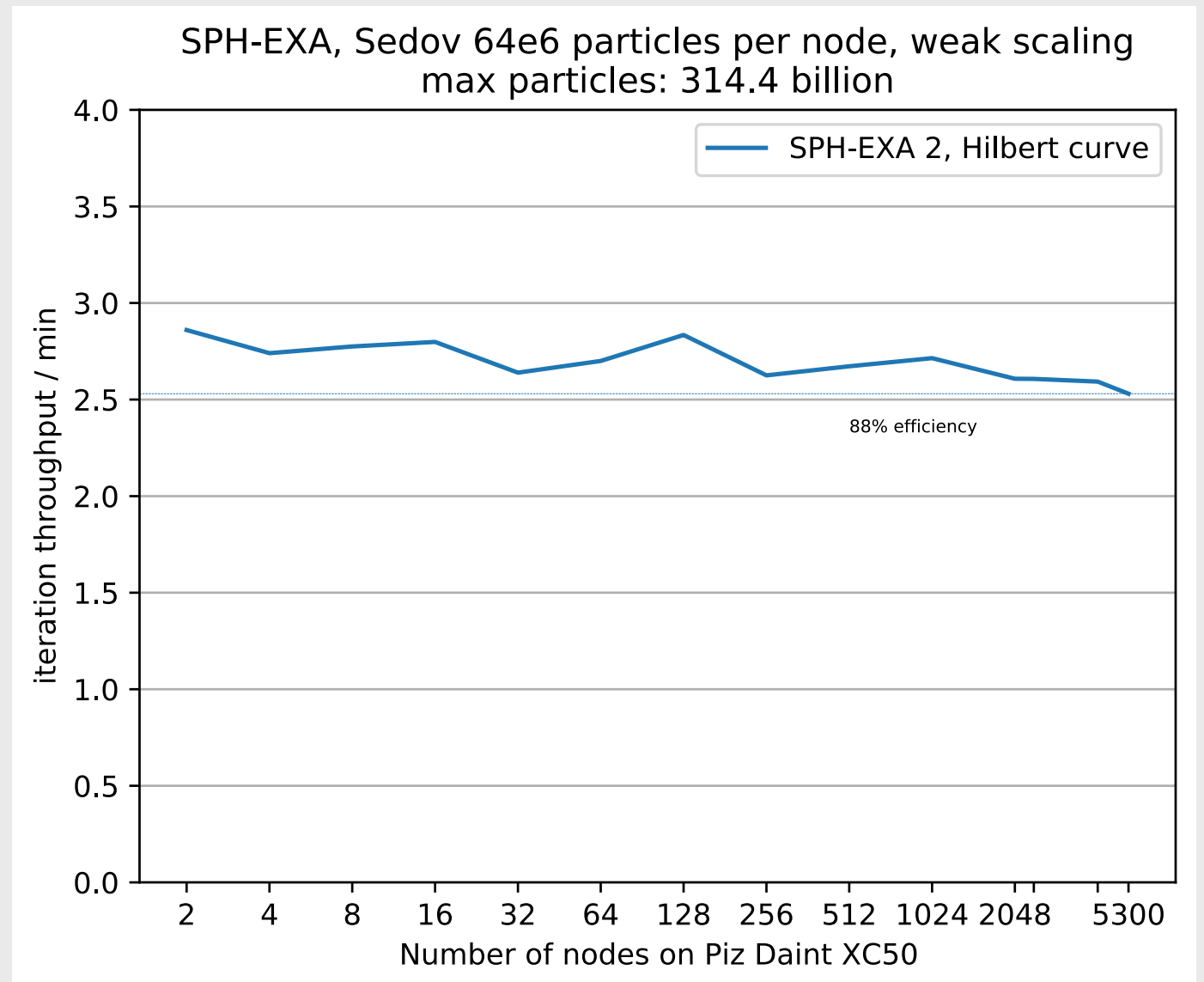
SPH performance, hydrodynamics only

Sedov blast wave on full Piz Daint

- **Performance is still continually being improved**

SPH-EXA, Sedov blast, weak scaling

93% efficiency
92% efficiency
58% efficiency

- SPH-EXA 2, current
- SPH-EXA 2, initial 07/2021
- SPH-EXA 1

iteration throughput / min

Number of nodes on Piz Daint XC50
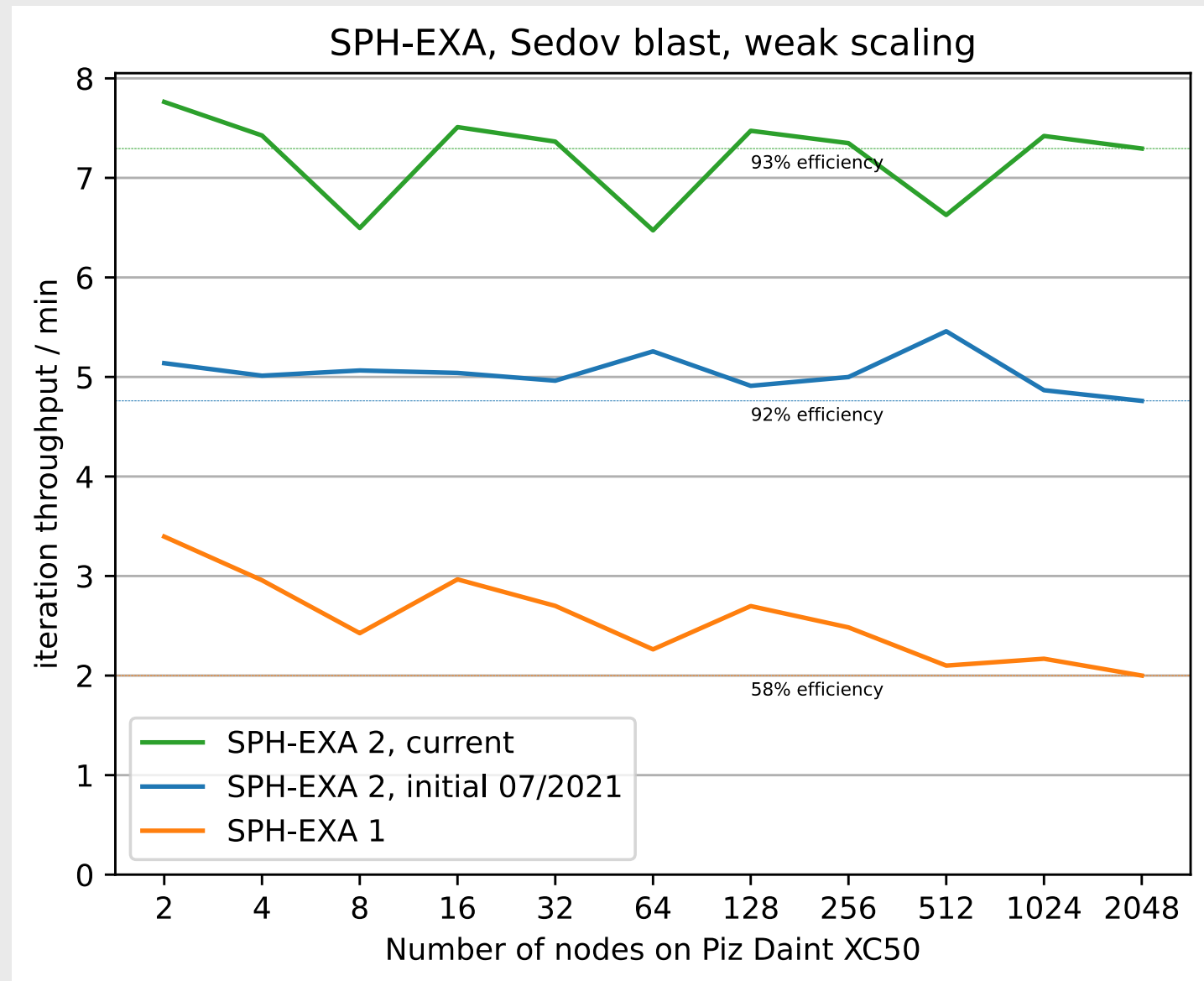
SPH-EXA: Hydrodynamics and gravity

Evrard collapse on Piz Daint

- **Testing absolute performance, multipole construction and exchange**

- **Scaling sucessfully test to ~1/2 of Piz Daint**

- **Can scale to ~1 trillion particles (Example here: 0.144 trillion particles full double precision. Corresponding to 0.314 on full machine.)**

SPH-EXA, Evrard collapse, up to 144 billion particles

weak scaling, theta = 0.5, 65.4M particles per node
gravity only

seconds per iteration — number of GPU nodes on Piz Daint

Universität Basel   Universität Zürich   CSCS   May 2022, Sebastian Keller