EIRON and EIRENE MsV Release

Huw Leggate
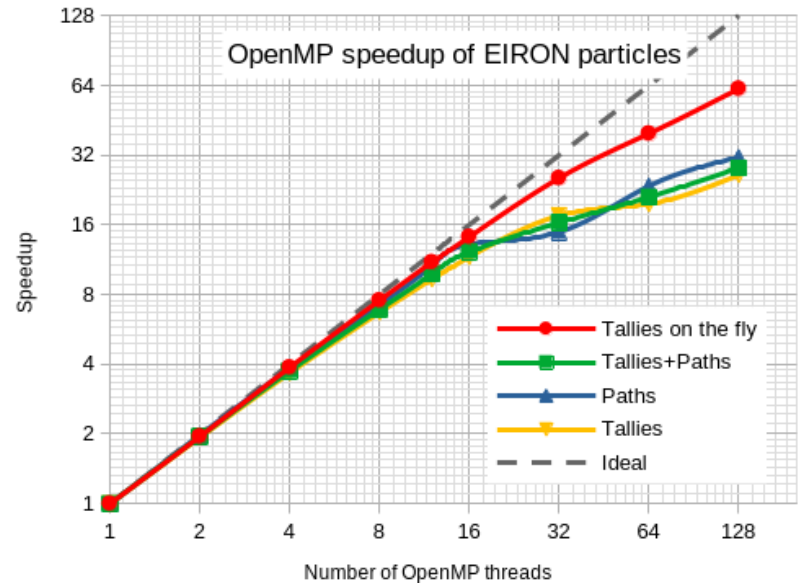
Dublin City University/Advanced Computing Hub - Garching

EUROfusion

DCU

Overview

- EIRON – EIRENE comparisons

- EIRENE MsV

  - OpenMP and final merge into develop

- Continuous Integration

  - OpenMP testing, optimisation

- Code improvements

  - Versioning, cmake, hooks, formatting

- Automated profiling

- ORB5 optimisation

EIRON-EIRENE Comparisons

- EIRON – Oskar Lappi

  - C++ code to test parallel schemes for EIRENE like problems

  - https://version.helsinki.fi/lapposka/eiron

  - No CRM

OpenMP speedup of EIRON particles

Legend:
- Tallies on the fly (red)
- Tallies+Paths (green)
- Paths (blue)
- Tallies (yellow)
- Ideal (dashed)

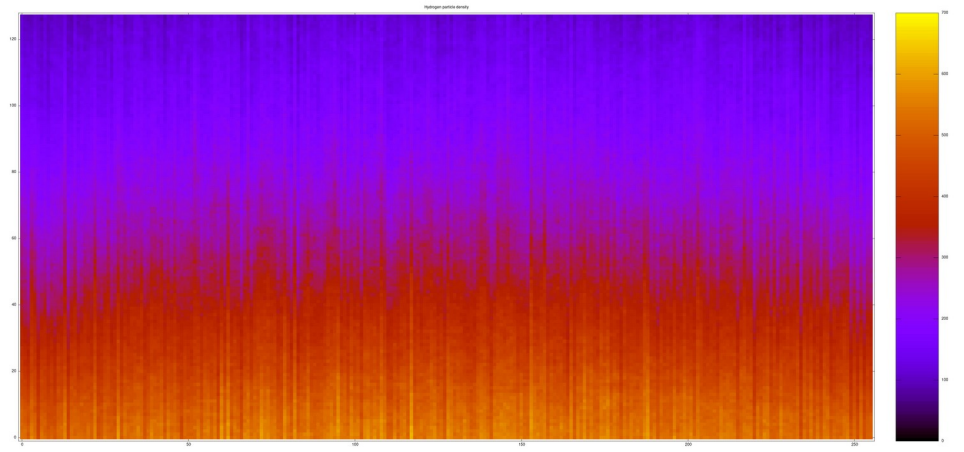X-axis: Number of OpenMP threads
Y-axis: Speedup

EIRON-EIRENE Comparisons

- Simple 2D slab case – 120000 particles
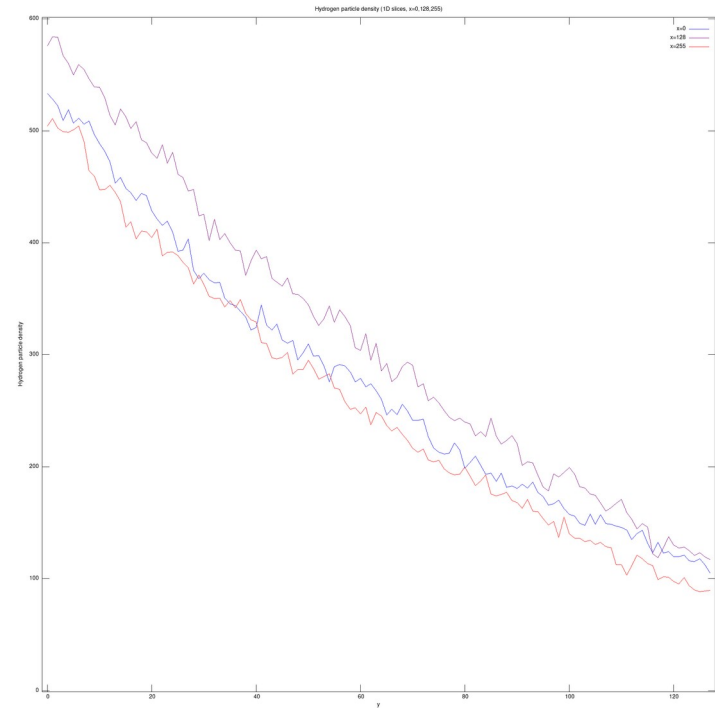
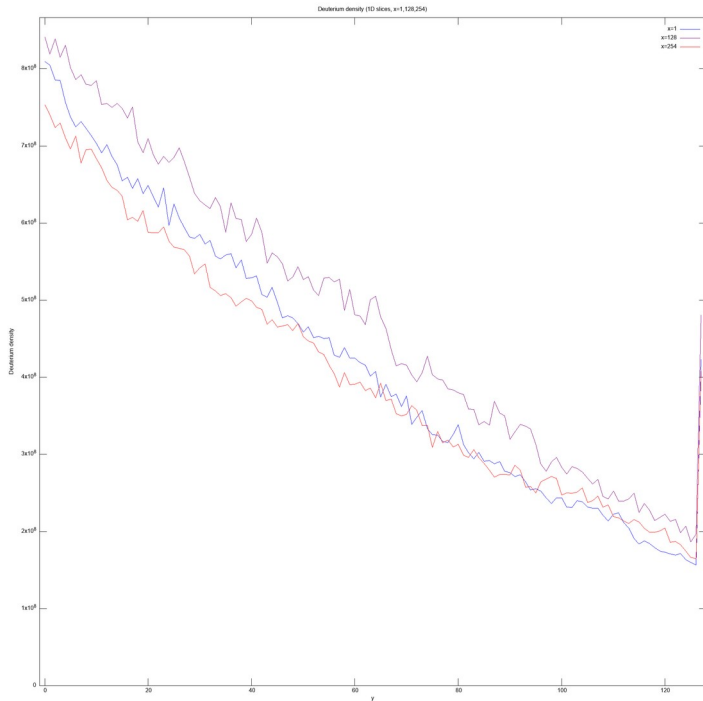- Constant angular distribution of injected particles
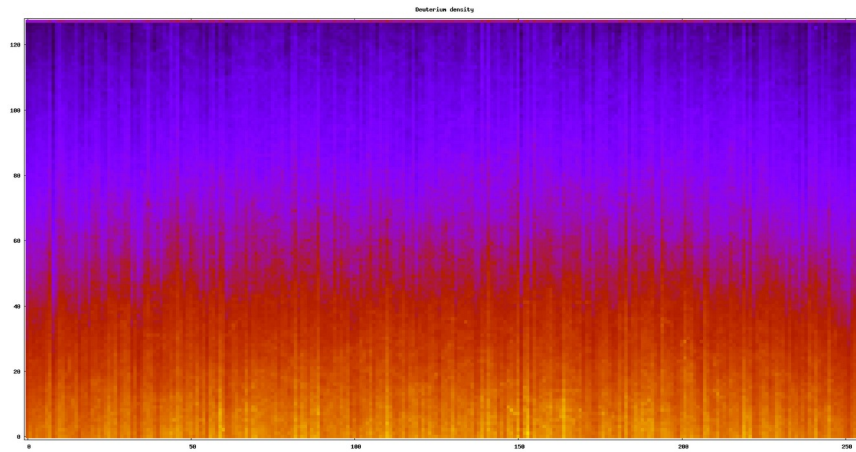
EIRENE

EIRON

# EIRON-EIRENE Comparisons

- Slices in x

EIRENE Milestone Version (MsV)

- Incorporated many large and small changes made over several years
  - JSON, AM Databases, OpenMP, licensing...
- Merge of branch eirene_unified into develop - March 29th 2023
- Bulk of work done by Petra Boerner
- > 2000 commits

Eirene OpenMP

- Initially implemented as part of HLST project in 2020
  - Remained in separate branch until now
  - Called from single or multiple threads using compile time switch
  - Modest speedup achieved ~5-10
  - ATOMIC statements limit scaling
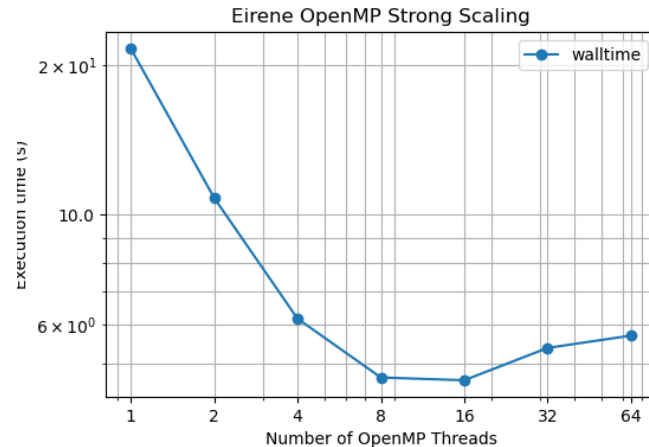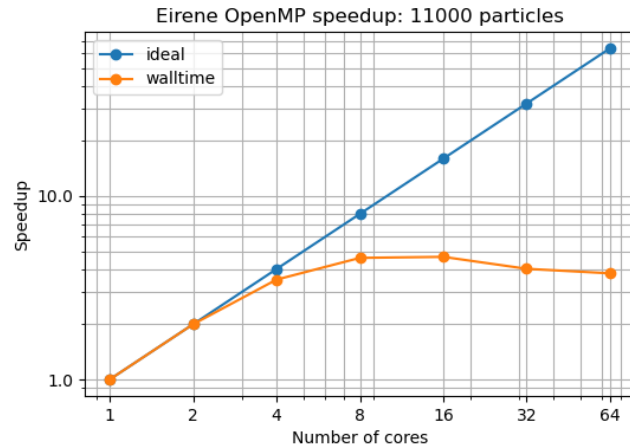
Continuous Integration
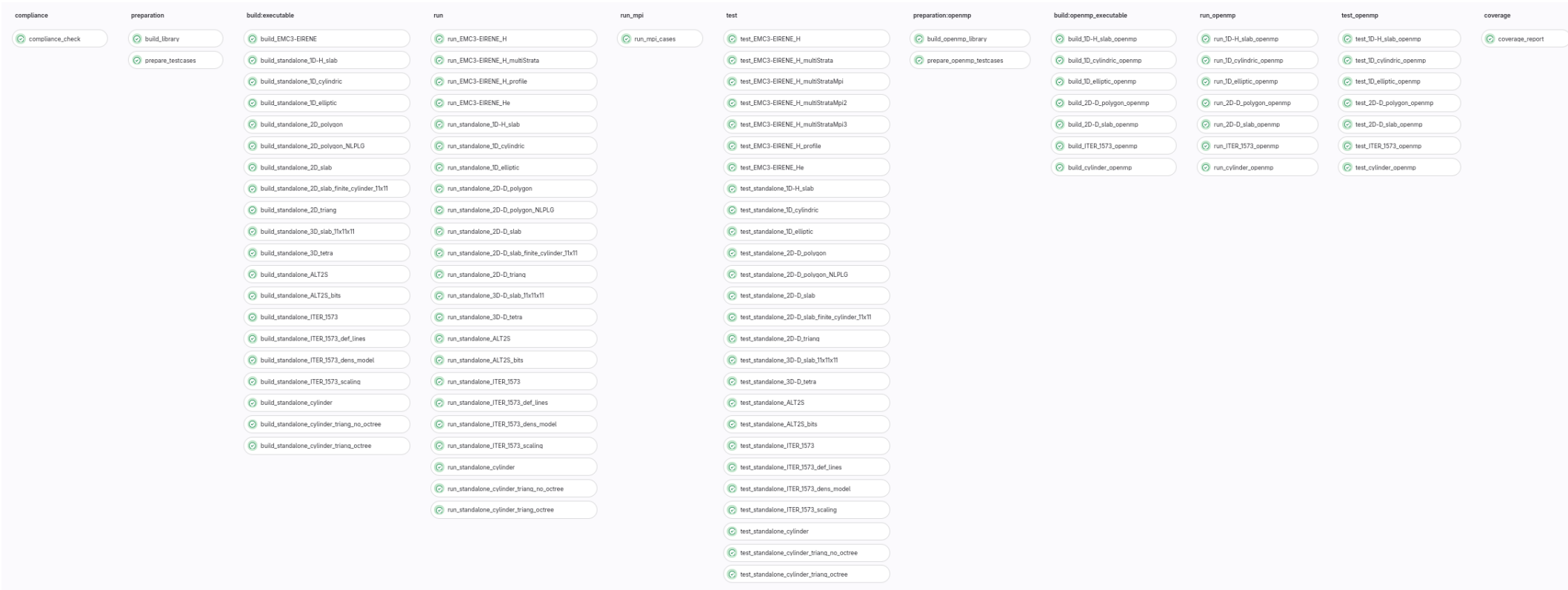
Continuous Integration

Compliance

Continuous Integration

Library compilation

Continuous Integration

Executable compilation
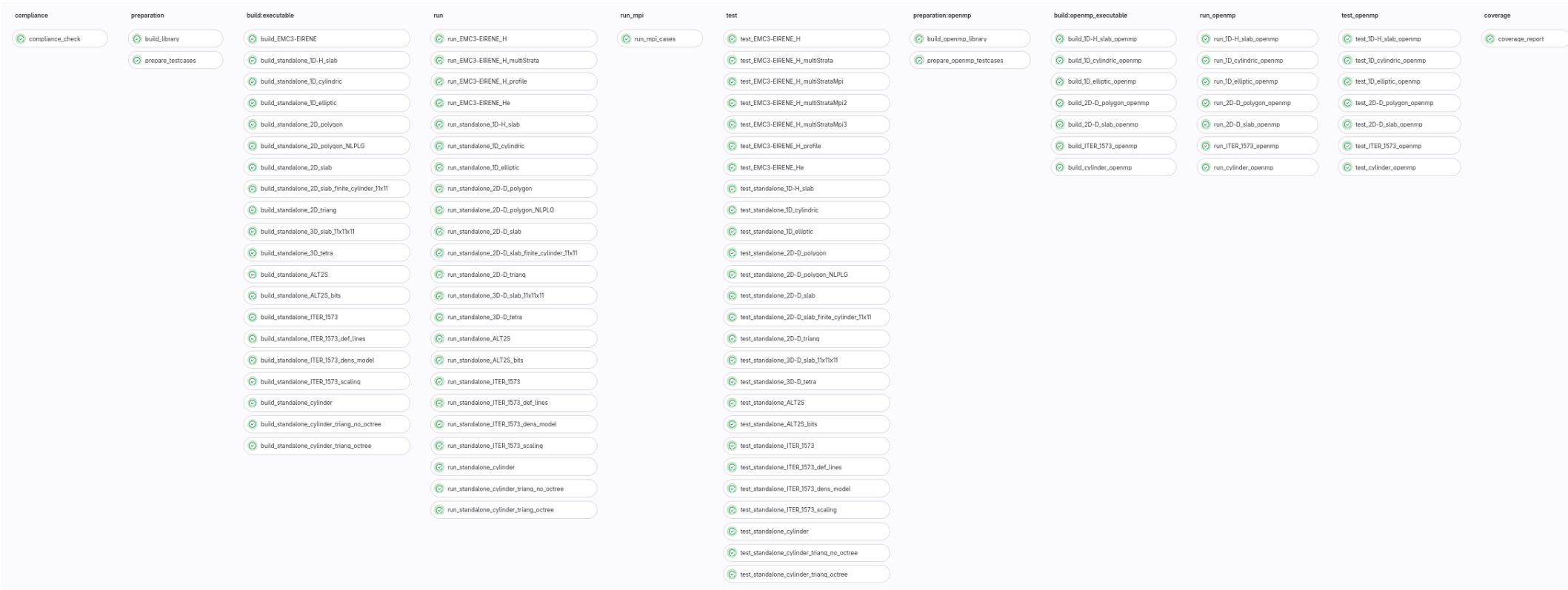
Continuous Integration

Serial execution

Continuous Integration

MPI execution

Continuous Integration

Comparison test

compliance	preparation	build:executable	run	run_mpi	test	preparation:openmp	build:openmp_executable	run_openmp	test_openmp	coverage
compliance_check	build_library	build_EMC3-EIRENE	run_EMC3-EIRENE_H	run_mpi_cases	test_EMC3-EIRENE_H	build_openmp_library	build_1D-H_slab_openmp	run_1D-H_slab_openmp	test_1D-H_slab_openmp	coverage_report
	prepare_testcases	build_standalone_1D-H_slab	run_EMC3-EIRENE_H_multiStrata		test_EMC3-EIRENE_H_multiStrata	prepare_openmp_testcases	build_1D_cylindric_openmp	run_1D_cylindric_openmp	test_1D_cylindric_openmp	
		build_standalone_1D_cylindric	run_EMC3-EIRENE_H_profile		test_EMC3-EIRENE_H_multiStrataMpi		build_1D_elliptic_openmp	run_1D_elliptic_openmp	test_1D_elliptic_openmp	
		build_standalone_1D_elliptic	run_EMC3-EIRENE_He		test_EMC3-EIRENE_H_multiStrataMpi2		build_2D-D_polygon_openmp	run_2D-D_polygon_openmp	test_2D-D_polygon_openmp	
		build_standalone_2D_polygon	run_standalone_1D-H_slab		test_EMC3-EIRENE_H_multiStrataMpi3		build_2D-D_slab_openmp	run_2D-D_slab_openmp	test_2D-D_slab_openmp	
		build_standalone_2D_polygon_NLPLG	run_standalone_1D_cylindric		test_EMC3-EIRENE_H_profile		build_ITER_1573_openmp	run_ITER_1573_openmp	test_ITER_1573_openmp	
		build_standalone_2D_slab	run_standalone_1D_elliptic		test_EMC3-EIRENE_He		build_cylinder_openmp	run_cylinder_openmp	test_cylinder_openmp	
		build_standalone_2D_slab_finite_cylinder_11x11	run_standalone_2D-D_polygon		test_standalone_1D-H_slab					
		build_standalone_2D_triang	run_standalone_2D-D_polygon_NLPLG		test_standalone_1D_cylindric					
		build_standalone_3D_slab_11x11x11	run_standalone_2D-D_slab		test_standalone_1D_elliptic					
		build_standalone_3D_tetra	run_standalone_2D-D_slab_finite_cylinder_11x11		test_standalone_2D-D_polygon					
		build_standalone_ALT2S	run_standalone_2D-D_triang		test_standalone_2D-D_polygon_NLPLG					
		build_standalone_ALT2S_bits	run_standalone_3D-D_slab_11x11x11		test_standalone_2D-D_slab					
		build_standalone_ITER_1573	run_standalone_3D-D_tetra		test_standalone_2D-D_slab_finite_cylinder_11x11					
		build_standalone_ITER_1573_def_lines	run_standalone_ALT2S		test_standalone_2D-D_triang					
		build_standalone_ITER_1573_dens_model	run_standalone_ALT2S_bits		test_standalone_3D-D_slab_11x11x11					
		build_standalone_ITER_1573_scaling	run_standalone_ITER_1573		test_standalone_3D-D_tetra					
		build_standalone_cylinder	run_standalone_ITER_1573_def_lines		test_standalone_ALT2S					
		build_standalone_cylinder_triang_no_octree	run_standalone_ITER_1573_dens_model		test_standalone_ALT2S_bits					
		build_standalone_cylinder_triang_octree	run_standalone_ITER_1573_scaling		test_standalone_ITER_1573					
			run_standalone_cylinder		test_standalone_ITER_1573_def_lines					
			run_standalone_cylinder_triang_no_octree		test_standalone_ITER_1573_dens_model					
			run_standalone_cylinder_triang_octree		test_standalone_ITER_1573_scaling					
					test_standalone_cylinder					
					test_standalone_cylinder_triang_no_octree					
					test_standalone_cylinder_triang_octree					

Continuous Integration

OpenMP

compliance	preparation	build:executable	run	run_mpi	test	preparation:openmp	build:openmp_executable	run_openmp	test_openmp	coverage
compliance_check	build_library	build_EMC3-EIRENE	run_EMC3-EIRENE_H	run_mpi_cases	test_EMC3-EIRENE_H	build_openmp_library	build_1D-H_slab_openmp	run_1D-H_slab_openmp	test_1D-H_slab_openmp	coverage_report
	prepare_testcases	build_standalone_1D-H_slab	run_EMC3-EIRENE_H_multiStrata		test_EMC3-EIRENE_H_multiStrata	prepare_openmp_testcases	build_1D_cylindric_openmp	run_1D_cylindric_openmp	test_1D_cylindric_openmp	
		build_standalone_1D_cylindric	run_EMC3-EIRENE_H_profile		test_EMC3-EIRENE_H_multiStrataMpi		build_1D_elliptic_openmp	run_1D_elliptic_openmp	test_1D_elliptic_openmp	
		build_standalone_1D_elliptic	run_EMC3-EIRENE_He		test_EMC3-EIRENE_H_multiStrataMpi2		build_2D-D_polygon_openmp	run_2D-D_polygon_openmp	test_2D-D_polygon_openmp	
		build_standalone_2D_polygon	run_standalone_1D-H_slab		test_EMC3-EIRENE_H_multiStrataMpi3		build_2D-D_slab_openmp	run_2D-D_slab_openmp	test_2D-D_slab_openmp	
		build_standalone_2D_polygon_NLPLG	run_standalone_1D_cylindric		test_EMC3-EIRENE_H_profile		build_ITER_1573_openmp	run_ITER_1573_openmp	test_ITER_1573_openmp	
		build_standalone_2D_slab	run_standalone_1D_elliptic		test_EMC3-EIRENE_He		build_cylinder_openmp	run_cylinder_openmp	test_cylinder_openmp	
		build_standalone_2D_slab_finite_cylinder_11x11	run_standalone_2D-D_polygon		test_standalone_1D-H_slab					
		build_standalone_2D_triang	run_standalone_2D-D_polygon_NLPLG		test_standalone_1D_cylindric					
		build_standalone_3D_slab_11x11x11	run_standalone_2D-D_slab		test_standalone_1D_elliptic					
		build_standalone_3D_tetra	run_standalone_2D-D_slab_finite_cylinder_11x11		test_standalone_2D-D_polygon					
		build_standalone_ALT2S	run_standalone_2D-D_triang		test_standalone_2D-D_polygon_NLPLG					
		build_standalone_ALT2S_bits	run_standalone_3D-D_slab_11x11x11		test_standalone_2D-D_slab					
		build_standalone_ITER_1573	run_standalone_3D-D_tetra		test_standalone_2D-D_slab_finite_cylinder_11x11					
		build_standalone_ITER_1573_def_lines	run_standalone_ALT2S		test_standalone_2D-D_triang					
		build_standalone_ITER_1573_dens_model	run_standalone_ALT2S_bits		test_standalone_3D-D_slab_11x11x11					
		build_standalone_ITER_1573_scaling	run_standalone_ITER_1573		test_standalone_3D-D_tetra					
		build_standalone_cylinder	run_standalone_ITER_1573_def_lines		test_standalone_ALT2S					
		build_standalone_cylinder_triang_no_octree	run_standalone_ITER_1573_dens_model		test_standalone_ALT2S_bits					
		build_standalone_cylinder_triang_octree	run_standalone_ITER_1573_scaling		test_standalone_ITER_1573					
			run_standalone_cylinder		test_standalone_ITER_1573_def_lines					
			run_standalone_cylinder_triang_no_octree		test_standalone_ITER_1573_dens_model					
			run_standalone_cylinder_triang_octree		test_standalone_ITER_1573_scaling					
					test_standalone_cylinder					
					test_standalone_cylinder_triang_no_octree					
					test_standalone_cylinder_triang_octree					

Continuous Integration - OpenMP

- Sample cases stored in EIRENE-SAMPLE-cases repository

- Serial and OpenMP use cases in different branches
  - Can be merged at any time

- OpenMP cases require synchronising of random seeds
  - Threads – Identical seeds for each thread processing N particles
  - Serial comparison – reseed with identical seed after every N particles

- OpenMP Reductions are non-associative
  - Small differences compared to serial

Continuous Integration - OpenMP

- Small differences require relative difference test

  - Python scripts replaces system diff for comparison test

- Sums resulting in result to close to zero present a problem

  - Serial $A \approx B$ $A - B \approx A * \varepsilon$ A and B do not change

  - OpenMP $A_1 \approx B_2$ $A - B \approx \pm A * \varepsilon$ A and B can vary by ε

- Can be a factor 2 difference

- Simplest approach to exclude affected values

    ~100 out of 30 million data points

CI Optimisation (w/D. Harting)

- Has grown over time ~ 90mins

  - Builds 23 standalone executables, 1 EMC3 coupled, 7 OpenMP

  - 26 Serial, 6 MPI, 7 OpenMP tests

- Has grown over time ~ 90mins

- Gitlab **dependencies** replaced with **needs**

- Shallow checkout of single commit of sample cases

  - Reduces

- Implementation of **rules** to control workflow

  - Sections can be disabled for development

Other code improvements

- Semantic versioning – Major.Minor.Patch

- Client side git hooks
    - Presently just pre-commit on version number and white space
    - Verified in CI

- cmake – automated search for JSON Libraries
    - This and similar applied to CRM module

- Formatting – fident (test – not applied)
    - EIRENE currently in mix of F90 free format and fixed format
    - fident used to convert – some adjustments needed by hand but works

EIRENE automated profiling

- Automatically produces MPI and OpenMP scaling

  - Based on shell scripts written by Oskar Lappi

  - Launches jobs and collects scaling data (JSON) for OpenMP and MPI

  - Produces a range of scaling plots
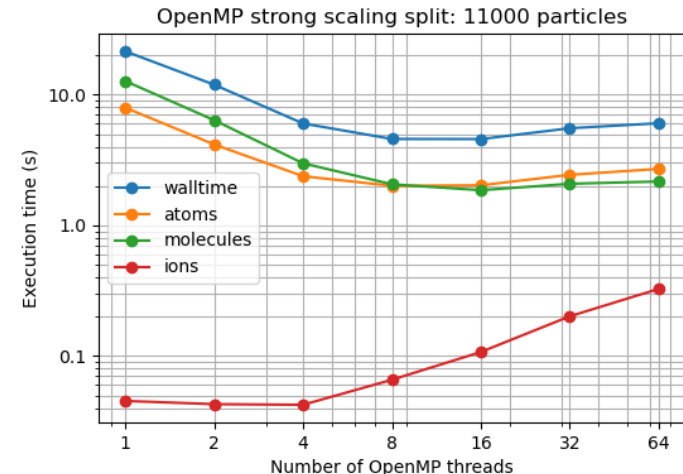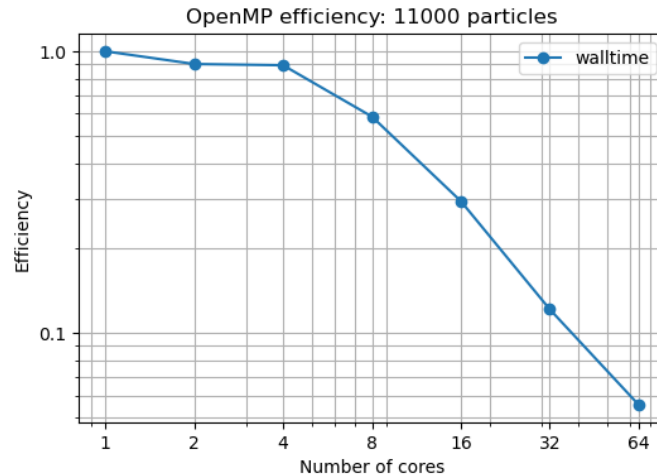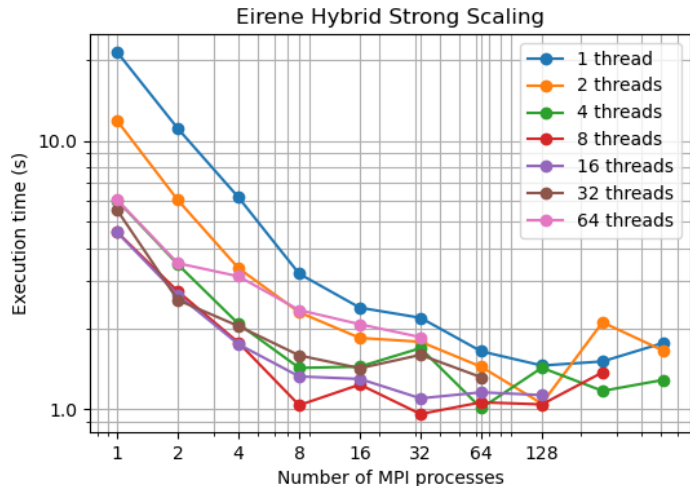
EIRENE automated profiling

- 5+1 Scripts – requires python jq
  - setup_profiling_run.sh
  - launch_jobs.sh
  - collect_profile_data.sh
  - plot_scaling.py
  - automation_script_header.sh
  - run_profiling.sh – runs all the scripts to produce scaling plots (30 mins)
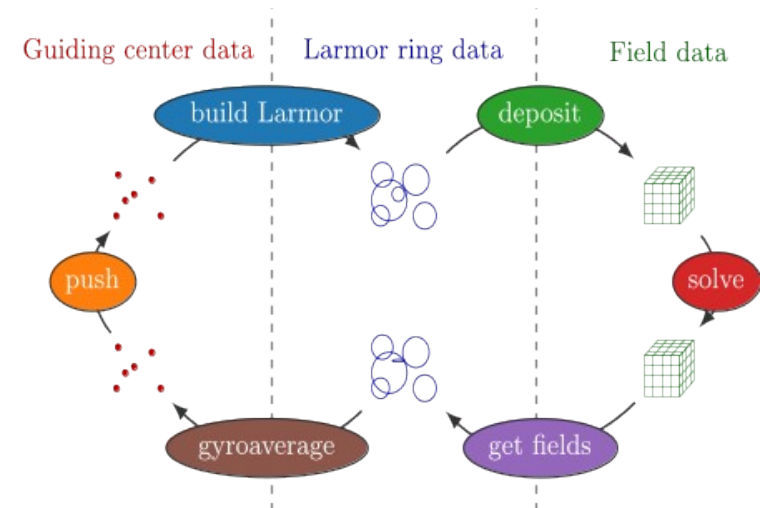- Some variables need to be set in the header

ORB5 memory optimisation

- Gyrokinetc δf simulation using OpenACC

  – Uses Larmor markers to gyroaverage and deposit charge

  – Memory footprint – 10^7 particles ~20 GB – (markers - 8 GB)

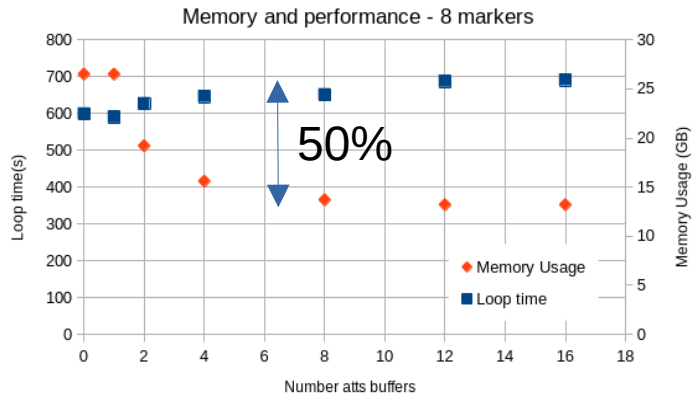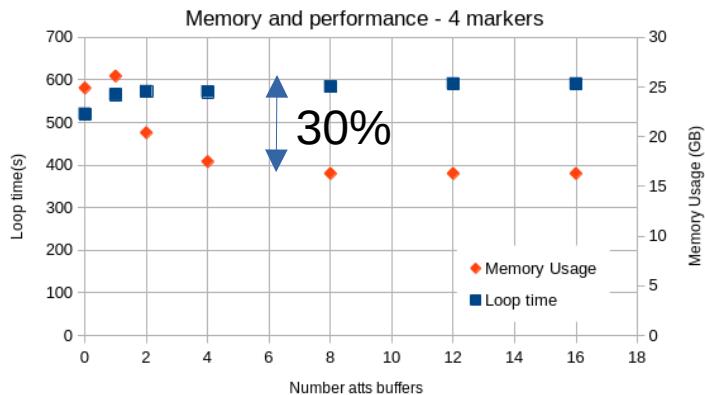- Optimisation reuses reduced marker arrays

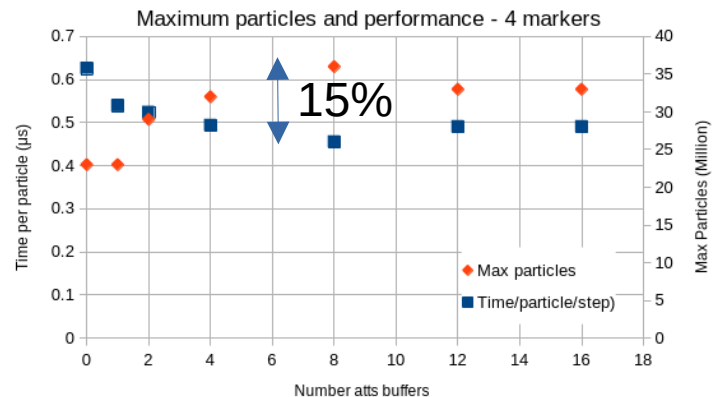Ohana 2021 https://doi.org/10.1016/j.cpc.2020.107208
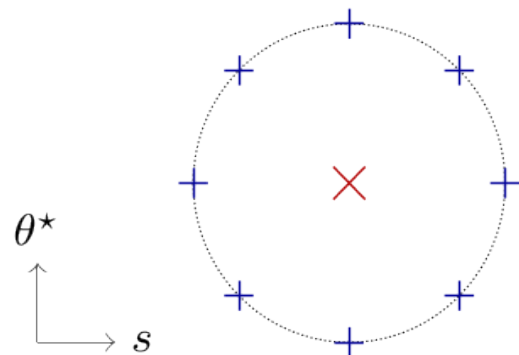
ORB5 memory optimisation

- 30%-50% reduction in memory – 10%-17% slowdown

- Allows more particles/GPU
  - 15% speedup per particle

Thank You

EIRENE CI status

- Current CI takes ~85mins – 5 stages

- Uses Debian 10 Buster (2019) in docker env

- Builds 18 standalone executables, 1 EMC3 coupled

- Runs 18 standalone test cases, 4 EMC3 cases, 6 MPI cases

- Runs seperate MPI tests

- Coverage report ~50%, failed on last instance

- OpenMP not yet included in develop

 – Duplicates existing serial CI cases

EIRENE CI status

- WIP_eirene_unified
  - New CI – Debian Bullseye
    - For Buster and Stretch compilation crashes
  - Also includes OpenMP tests
  - Includes flags for turning off stages
    - INCLUDE_SERIAL
    - INCLUDE_OPENMP
    - INCLUDE_MPI
    - INCLUDE EMC3

O-EIRENE – Continuous Integration

- EIRENE uses a Continuous Integration Pipeline on Gitlab (YAML)

Build Libraries

Build Test Cases

Run Test Cases

Run Special Cases (MPI)

Verify Test Cases
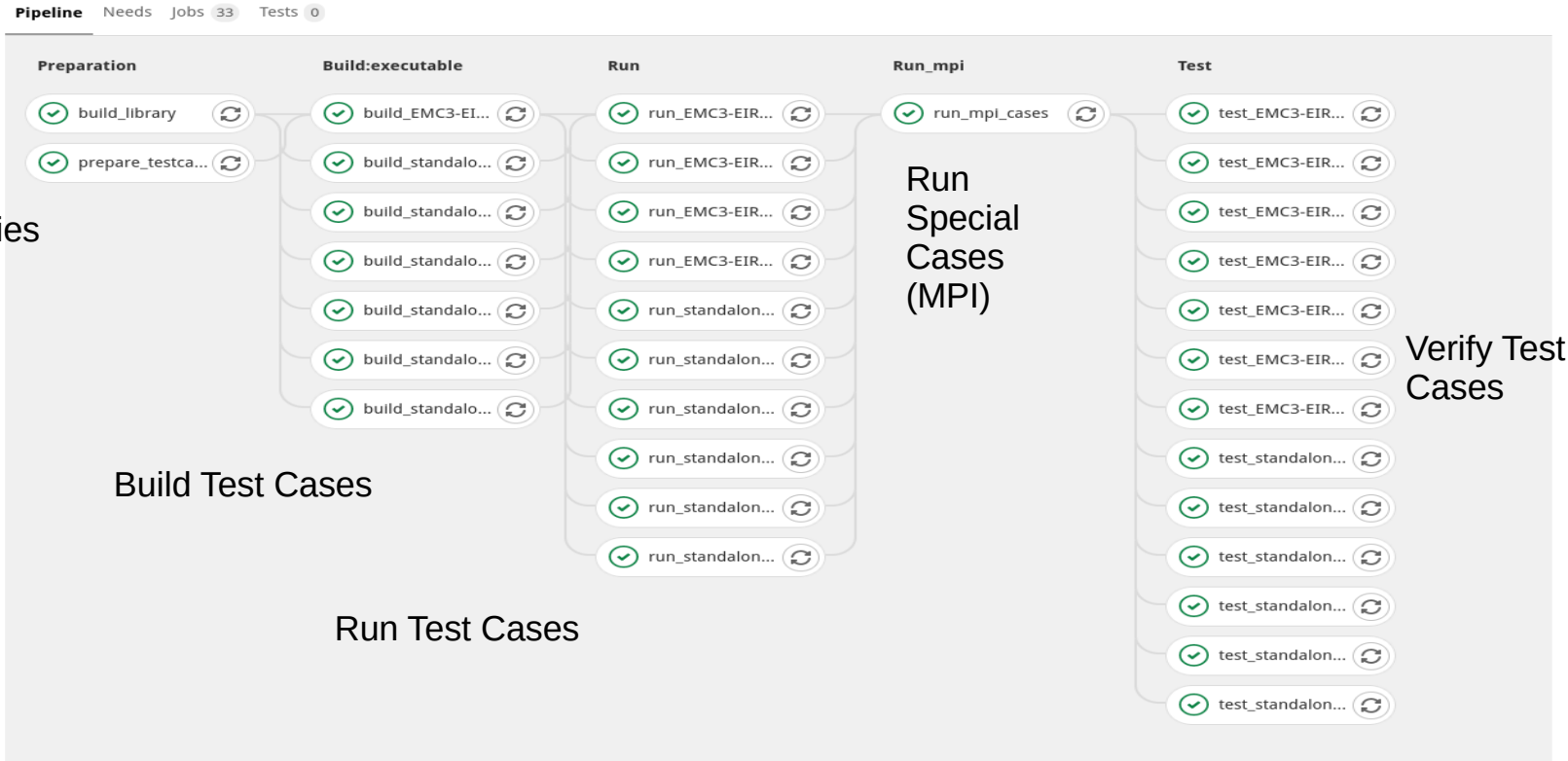
O-EIRENE – Continuous Integration

- Stage for OpenMP being developed – additional stages

OpenMP stages

- Duplication of stages retains CI on non-OpenMP code