Project NEPTUNE

Work Package 2: Fluid Referent Models

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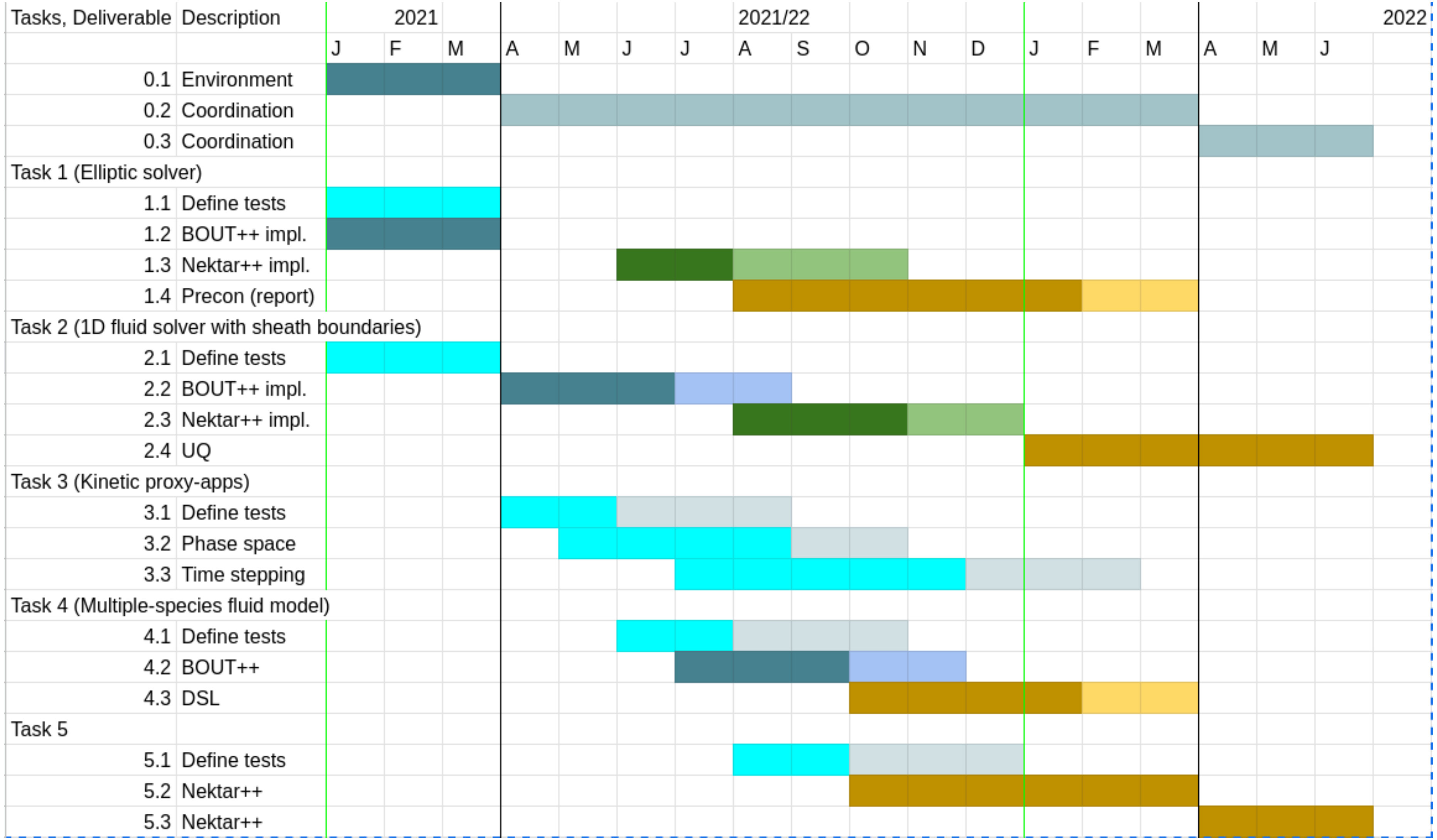
Met Office

UK Research and Innovation

UK Atomic Energy Authority

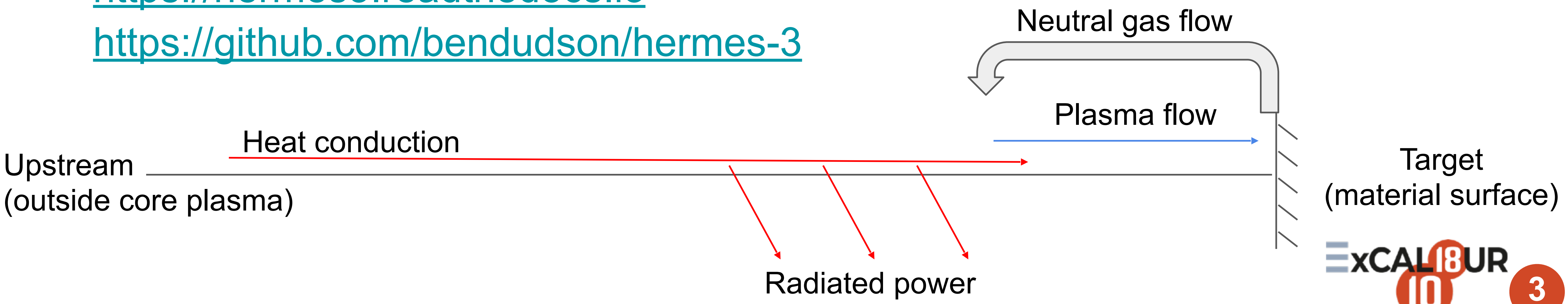
Overall Project Timeline



1D Fluid Model
SD1D

Using SD1D and Hermes-3, built on BOUT++, to develop tests and examples

- **SD1D**, a 1D model of hydrogen plasmas https://doi.org/10.1088/1361-6587/ab1321 https://github.com/boutproject/SD1D/
- **Hermes-3**, a 1D/2D/3D multi-species model under development https://hermes3.readthedocs.io https://github.com/bendudson/hermes-3

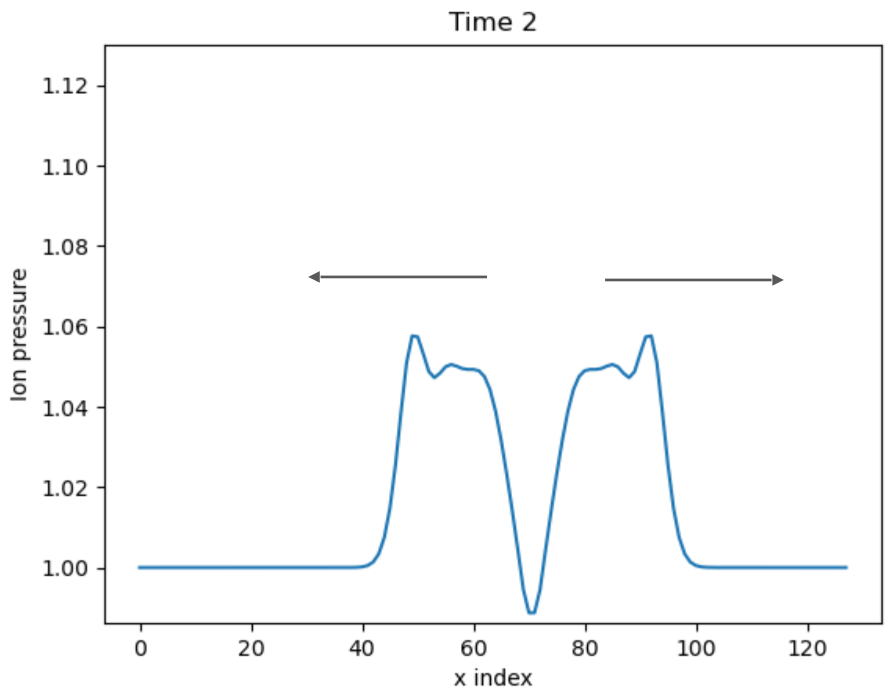


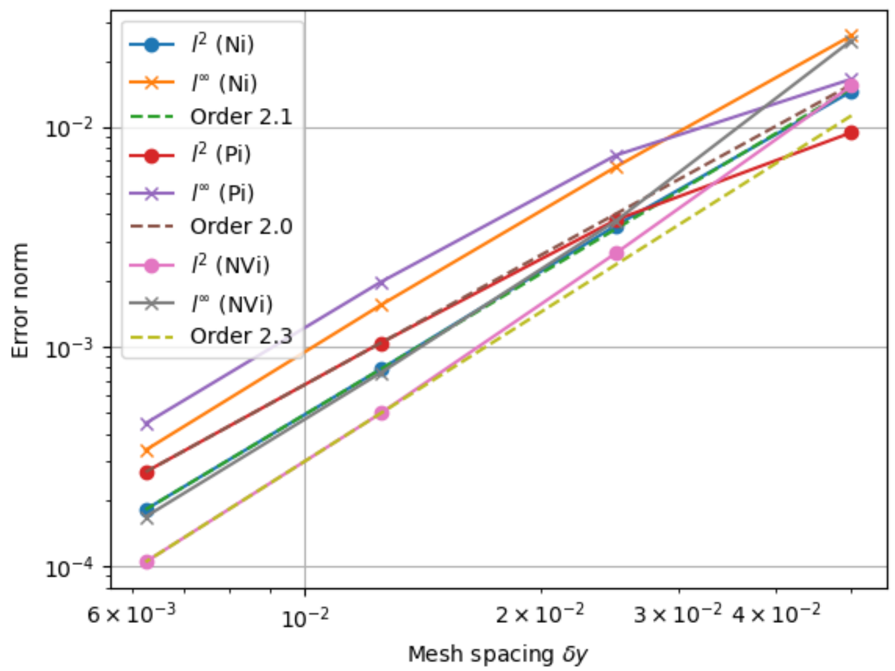
1D Fluid Model

Component Tests

Check individual parts of the model

- 1D fluid flow, periodic domain. MMS convergence test
  https://github.com/bendudson/hermes-3/tree/master/tests/integrated/1D-fluid





1D Fluid Model

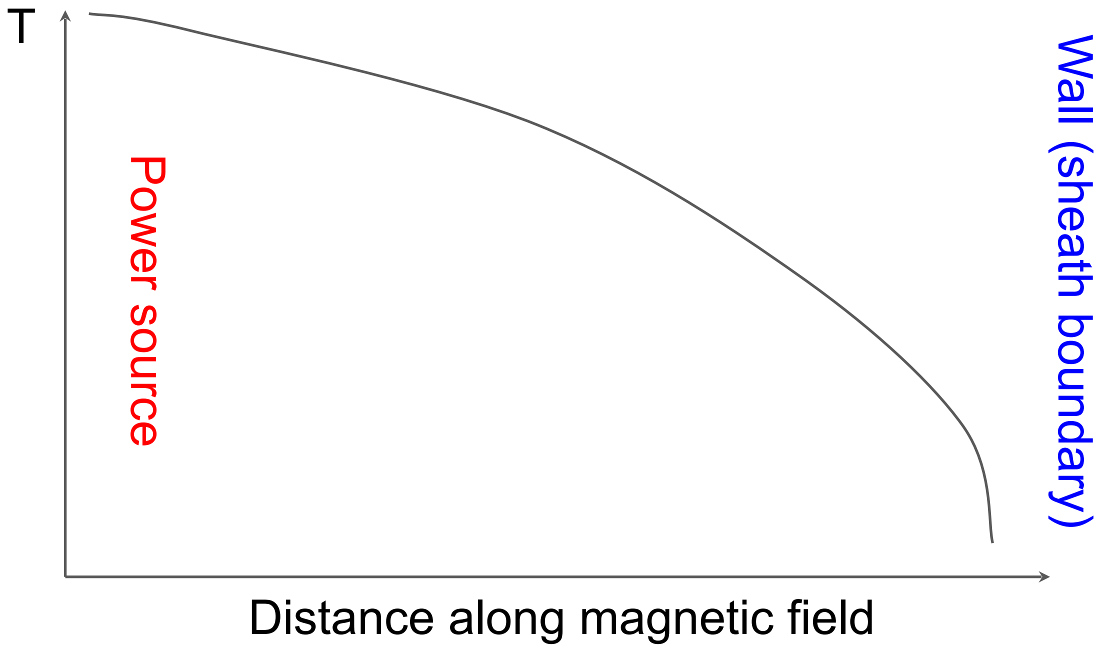
Component Tests

Check individual parts of the model

- 1D fluid flow, periodic domain. MMS convergence test
  https://github.com/bendudson/hermes-3/tree/master/tests/integrated/1D-fluid

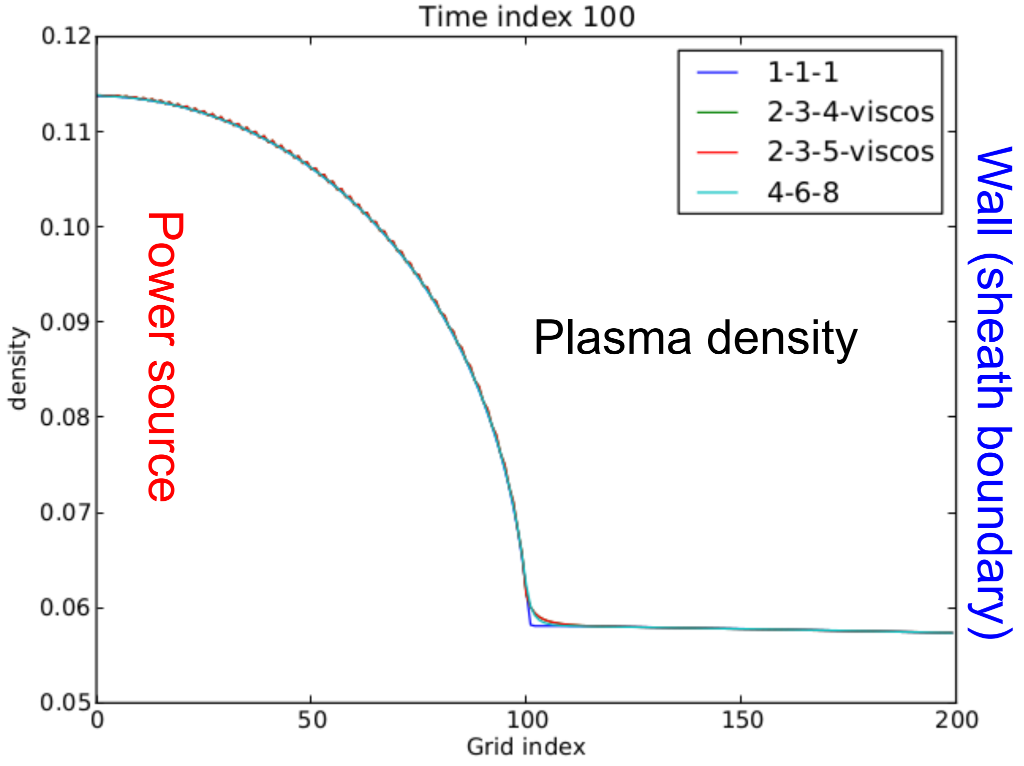
- Nonlinear heat conduction
  Analytic solution (2-point model)

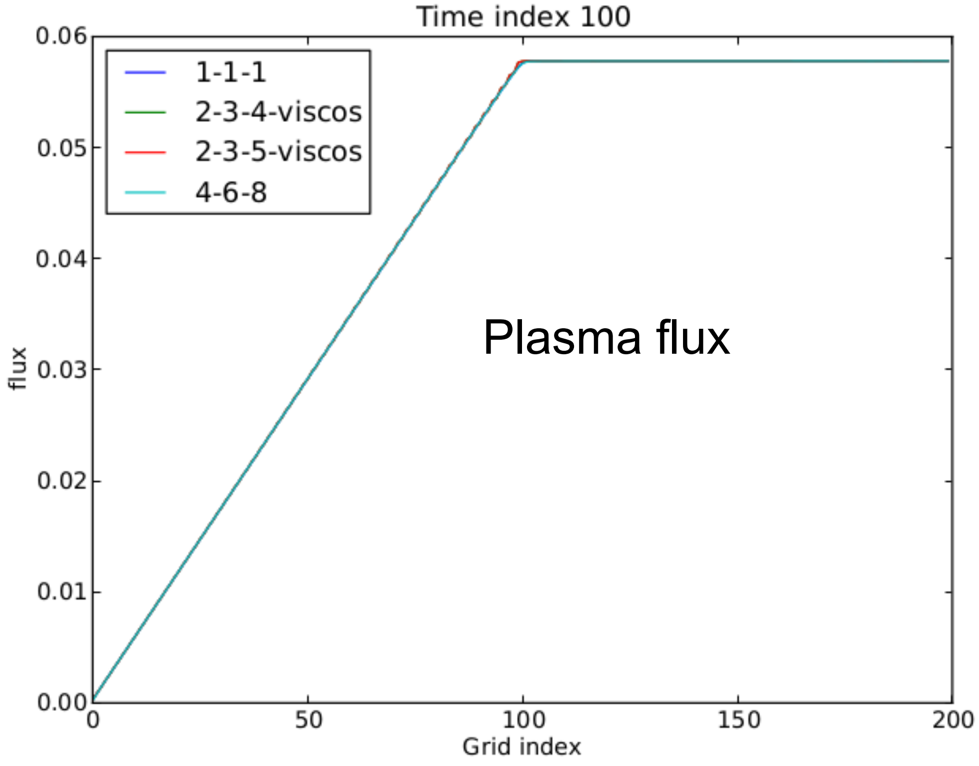
- Conservation checks
  E.g. particle balance in a closed system



1D Fluid Model
Sources

- Outflow boundary conditions on one side, no-flow on the other
- Source over part of the domain -> Sharp changes in gradients



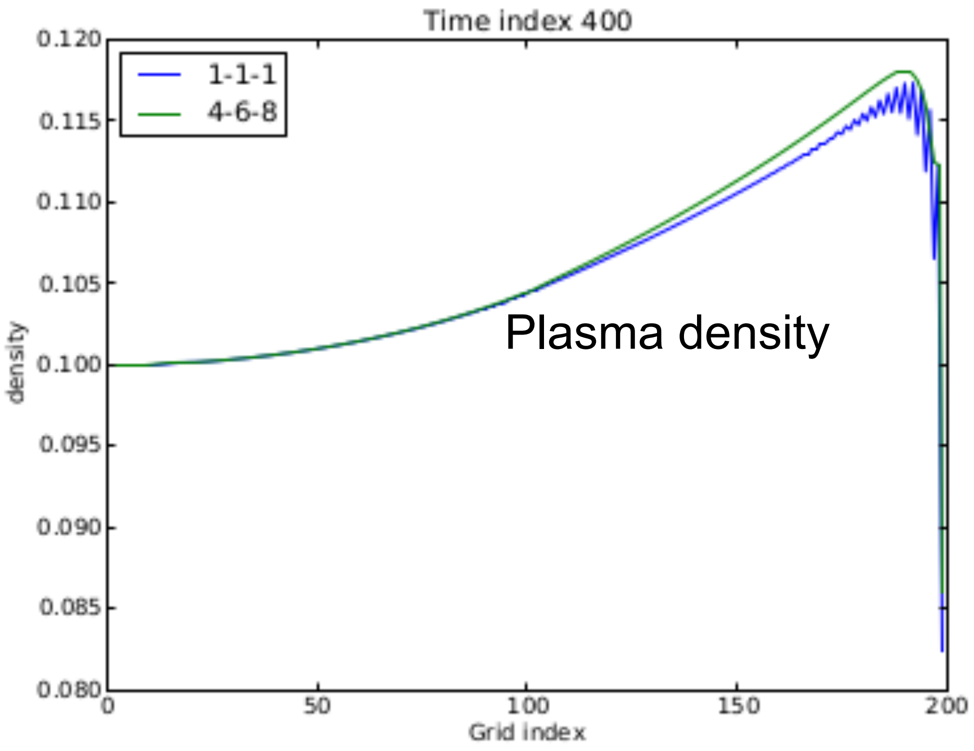


1D Fluid Model

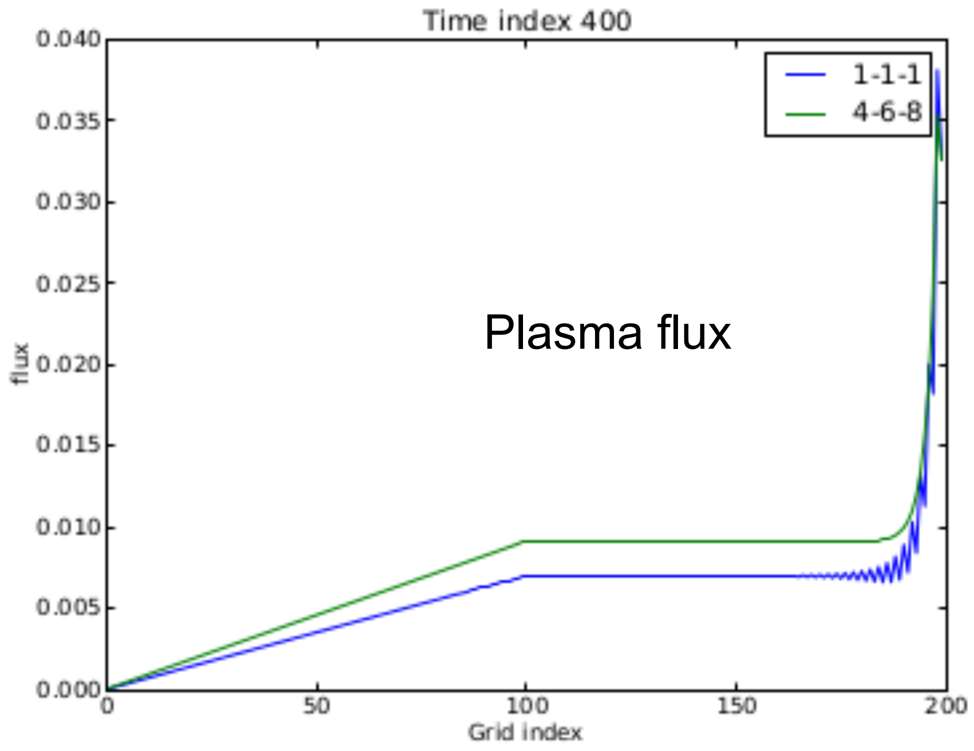
Boundary Conditions

Sheath boundary conditions (sound speed)

recycling of plasma -> neutral gas -> plasma (atomic reactions)



(a) Density n



(b) Flux $nV_{||}$

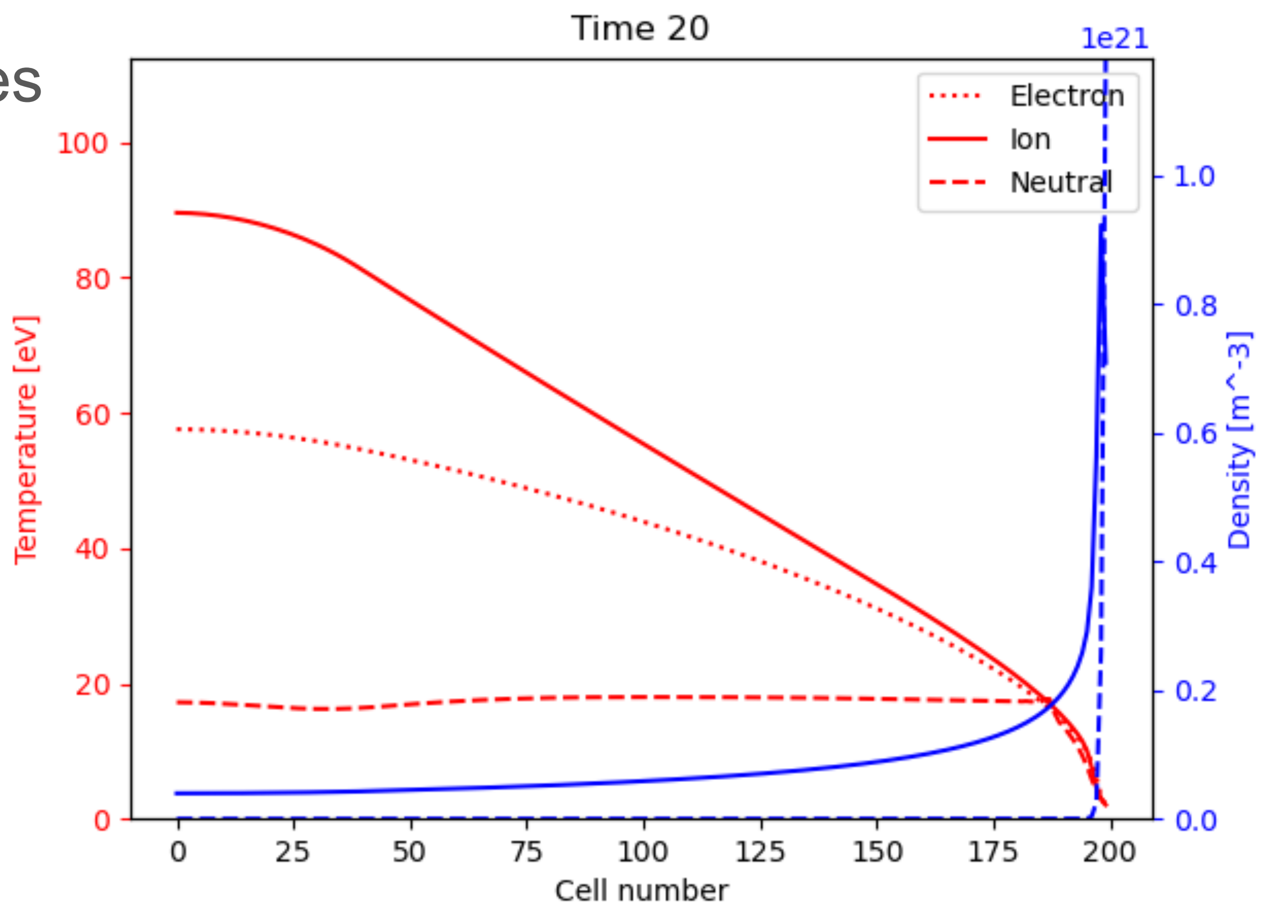
1D Fluid Model

Multi Species

- Separate ion and electron temperatures
- Coupling (collisions) between species

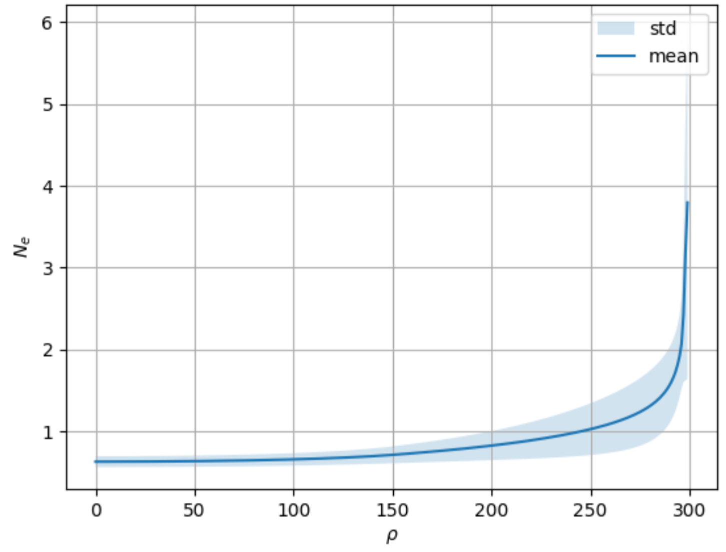
- Extension to multiple ion species
  D, T, He, Be, W, Ne, Ar, …

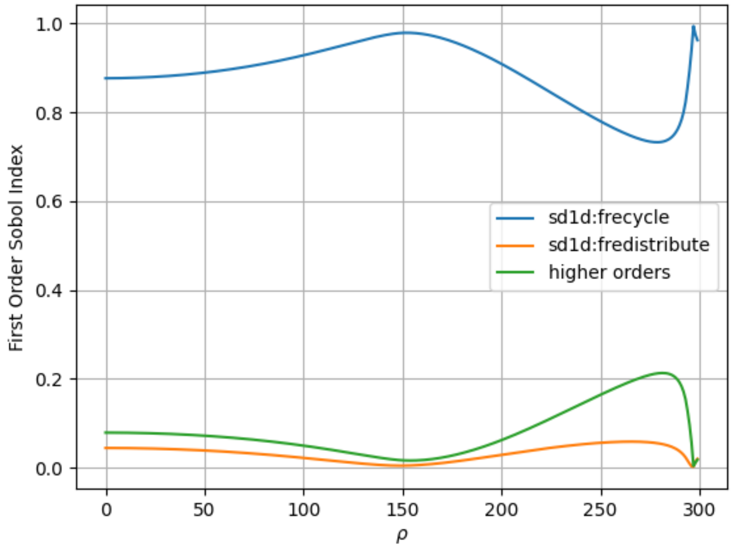
- Reactions and collisions between species



1D Fluid Model

UQ





- Developed example implementations of non-intrusive UQ workflows using EasyVVUQ with SD1D.
- Explore role of uncertainty in upstream sources and downstream boundary conditions.
- Helps identify key parameters to refine in order to reduce key uncertainties.

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Work Package 4: Support and Coordination

Steven Wright, Ben Dudson, Peter Hill, David Dickinson, Edward Higgins, Chris Ridgers

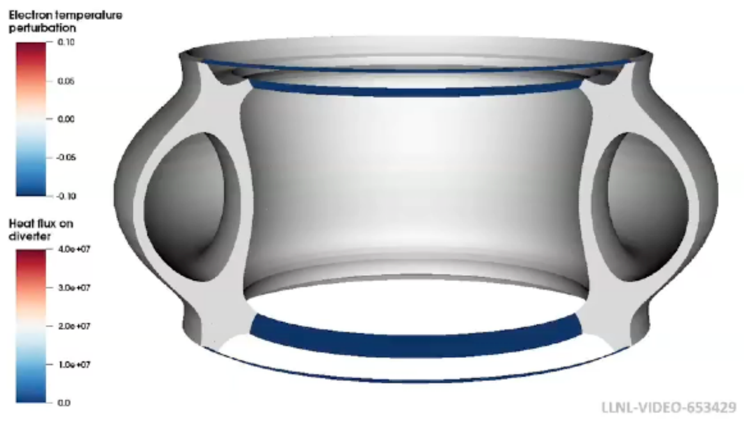
University of York

Gihan Mudalige, Tom Goffrey, Ben McMillan

University of Warwick

Project NEPTUNE

NEutrals & Plasma TUrbulence Numerics for the Exascale



NEKTAR++
SPECTRAL/HP ELEMENT FRAMEWORK

EPOCH

- **WP1 Numerical Representation**
  - **Algorithms, coupling between WP2 and WP3**
- **WP2 Plasma Multi Physics Model**
  - **Fluid models for plasma edge**
- **WP3 Neutral Gas & Impurity Model**
  - **Particle models for region outside and just inside the plasma**
- **WP4 Code Structure & Coordination**
  - **Best practices in engineering a *Performance Portable* Exascale-ready code**

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FM-WP4 Code Structure and Coordination

Funded Projects

Our work has been funded by two projects (so far):

- **Investigate DSL and Code Generation Techniques (Jan 2021 — Sept 2021)**
- **Support and Coordination (Jan 2022 — Dec 2022)**
- **Software Support Procurement (Sept 2022 — Feb 2024)**

FM-WP4 Code Structure and Coordination

Investigate DSL and code generation techniques

Our first project was based around four deliverables:

- **Survey of available (and upcoming) technologies**
- **Identification of representative applications**
- **Evaluation of approaches to performance portability for Fusion applications**
- **Identification of best practices**

FM-WP4 Code Structure and Coordination

Support and Coordination

Our second project was also based around four deliverables:

- **Periodic revision of Hardware and Software Reviews**
- **Development of an FEM-PIC mini-application**
- **Performance evaluation of FEM-PIC application**
- **Outline proposal for a particle-methods DSL**

FM-WP4 Code Structure and Coordination

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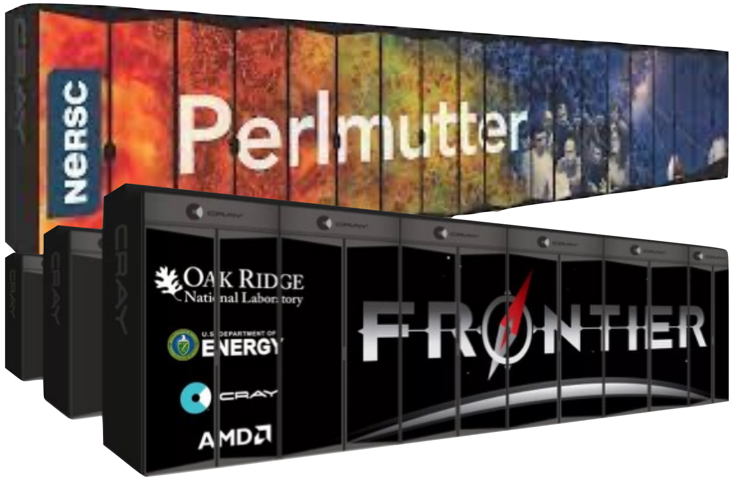
Context

Pre- and Post-Exascale Hardware

- All pre- and post-Exascale systems will be heterogenous (… except Fugaku)
- Most of the FLOP/s will be provided by GPU accelerators
    - NVIDIA Hopper
    - AMD Instinct
    - Intel Xe
- Most systems will use x86_64 hosts from Intel and AMD
  (+ perhaps some NVIDIA Grace)

Context

Pre- and Post-Exascale Hardware



DoE have 4 Cray Shasta systems installed or in development

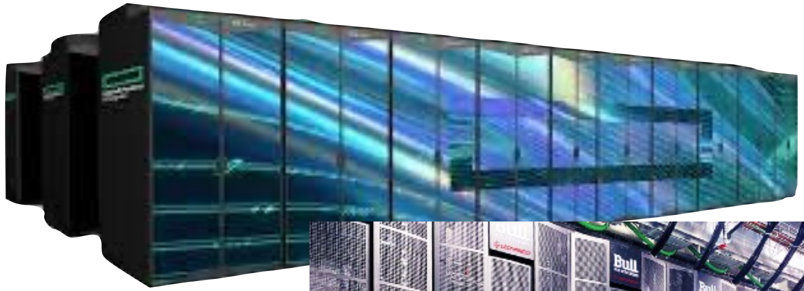
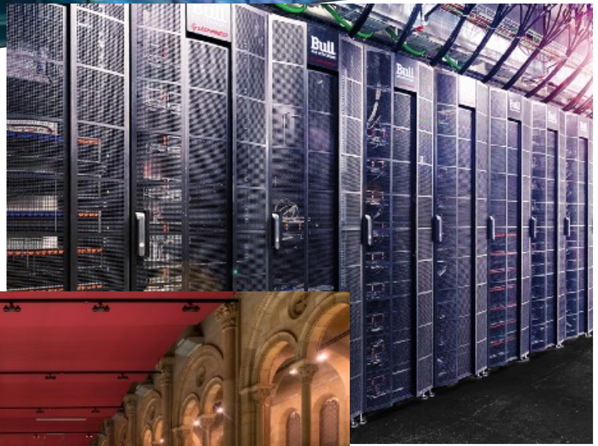
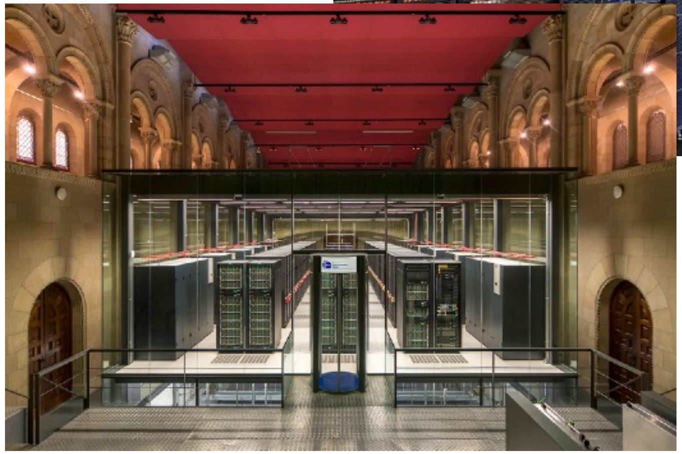
- Perlmutter
  - 70.87 PFLOP/s (achieved… so far!)
  - AMD EPYC CPUs (Milan) with NVIDIA A100 GPUs
- Frontier
  - 1.1 EFLOP/s 🎉 🎉 🎉 (achieved)
  - AMD EPYC CPUs (Trento) with AMD Instinct (MI250X) GPUs
- Aurora (To Appear)
  - >1 EFLOP
  - Intel Xeon CPUs (Sapphire Rapids) with Intel Xe (PV) GPUs
- El Capitan (To Appear)
  - 2+ EFLOP/s
  - AMD EPYC CPUs (Genoa) with AMD Instinct GPUs

Context

Pre- and Post-Exascale Hardware

Europe has 3 pre-Exascale systems in development

- LUMI
  - 151 PFLOP/s (Achieved)
  - AMD EPYC (Trento) CPUs with AMD Instinct (MI250X) GPUs
- LEONARDO
  - 300+ PFLOP/s
  - Intel Xeon CPUs (Sapphire Rapids) with NVIDIA A100 GPUs
- MareNostrum 5
  - 300+ PFLOP/s
  - 4 distinct PFLOP/s systems
    - Intel Xeon CPUs (Sapphire Rapids) with NVIDIA H100 GPUs
    - Intel Xeon CPUs (Emerald Rapids) with Rialto Bridge GPUs
    - Intel Xeon CPUs (Sapphire Rapids)
    - NVIDIA Grace Superchips

Context

Pre- and Post-Exascale Hardware

The UK

- ARCHER-2
  - ~28 PFLOP/s
  - AMD EPYC CPUs
- Isambard
  - ARM CPUs (ThunderX2 and A64FX)
  - AMD EPYC CPUs
  - Intel Xeon CPUs
  - IBM Power9 CPUs
  - NVIDIA P100 and NVIDIA V100 GPUs
- Viking, Avon, Bede, etc

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Context

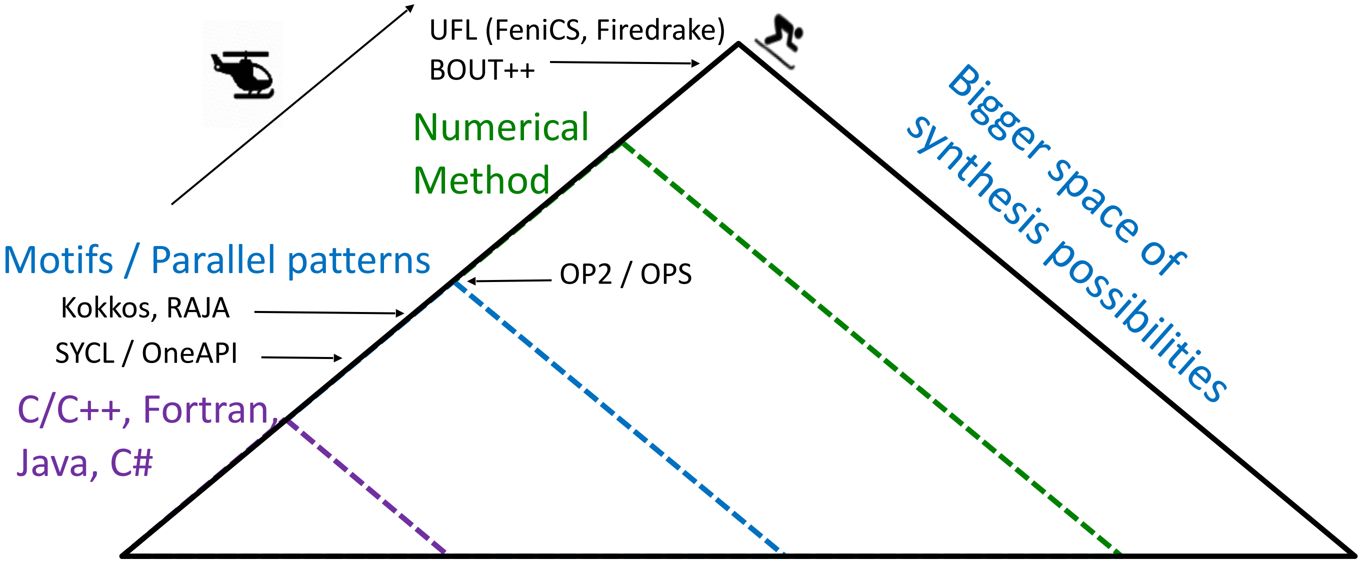
Software Approaches to Exascale

- Proliferation of Parallel programming models and software
- Open standards
  - Directives – OpenMP, OpenACC
  - OpenCL and SYCL
- Proprietary models
  - Almost as if each vendor introduces their own proprietary model
  - NVIDIA - OpenACC, CUDA
  - AMD - HIP/ROCm
  - Intel - OneAPI (SYCL + Intel specific software)
- Template libraries
  - Kokkos and RAJA (championed by the DoE labs)

Context

Software Approaches to Exascale

- **Domain Specific Languages**
  - **Code-gen from mathematical equations - Bout++, FeniCS, Firedrake, Devito**
  - **Parallel patters/motifs based Code-gen - OP2/OPS**



Adapted from: *Synthesis versus Analysis: What Do We Actually Gain from Domain-Specificity?* Keynote talk at the LCPC 2015. Paul H. J. Kelly (Imperial College London)

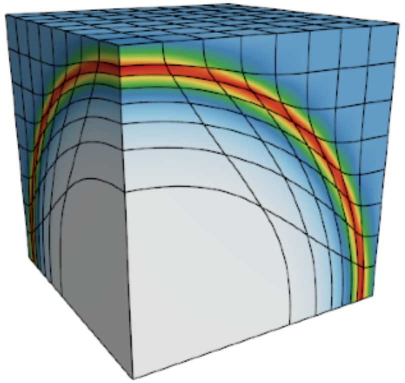
Applications for Evaluation

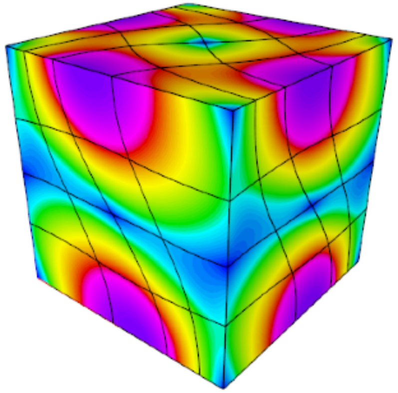
Identification of representative proxy applications

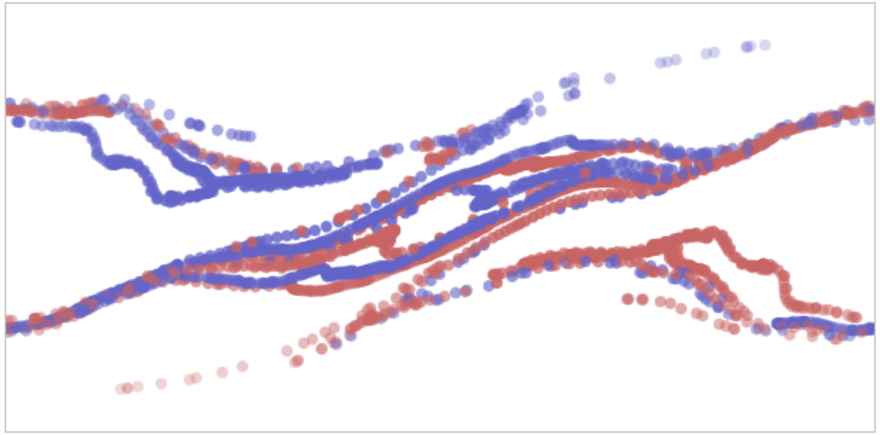
- NEPTUNE requires both Fluid and Particle models
- BOUT++/Nektar/EPOCH are likely too large to evaluate for portability
- Our evaluation is based on mini-applications that implement similar schemes
    - Finite Differencing
    - Finite Element Method
    - High-order FEM
    - Particle-in-Cell

Applications for Evaluation

Identification of representative proxy applications







- Fluid Codes
  - HEAT — Finite difference mini-app
  - TEALEAF – Finite difference mini-app
  - MINIFE – Finite element mini-app
  - LAGHOS – High-order FEM mini-app
- Particle Codes
  - CABANAPIC – structured PIC demonstrator
  - VPIC – Vectorised, structured PIC code
  - EMPIRE-PIC – Unstructured FEM-PIC code
- … plus more apps to be added!

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Evaluation Methodology

A Metric for Performance Portability

- **Evaluation based on Pennycook et al.'s metric [1]**

$$\text{Ᵽ}(a,p,H) = \begin{cases} \dfrac{|H|}{\displaystyle\sum_{i \in H} \frac{1}{e_i(a,p)}} & \text{if } i \text{ is supported } \forall i \in H \\ 0 & \text{otherwise} \end{cases}$$

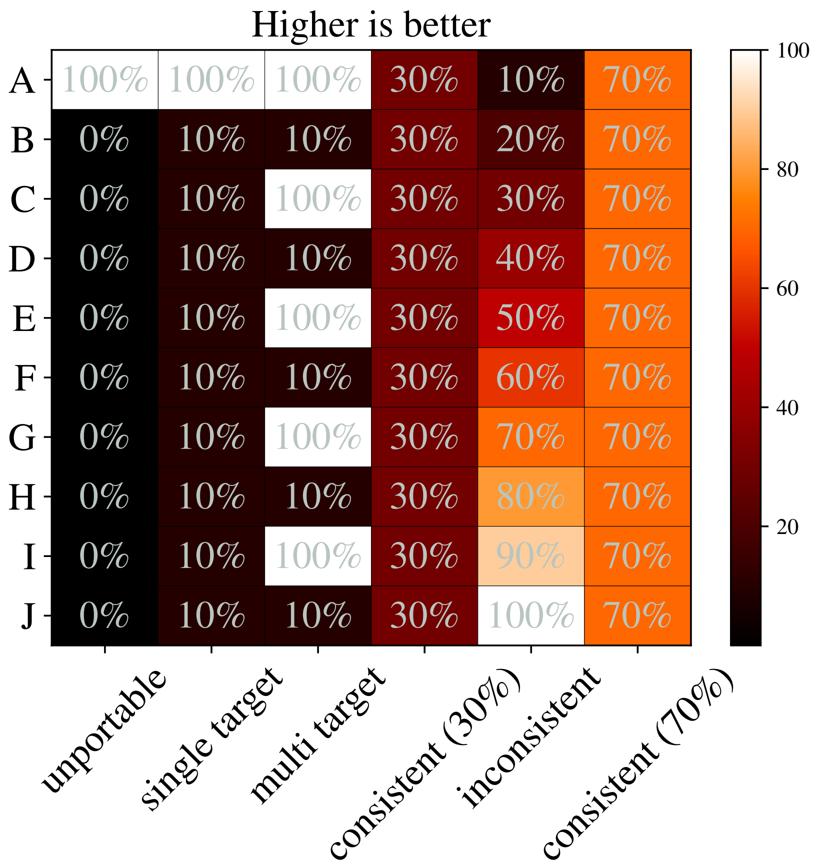
- **Find harmonic mean of applications performance efficiency**
  - **Application efficiency – achieved performance / best recorded performance**
  - **Architectural efficiency – achieved performance / theoretical max**

[1] S.J. Pennycook, J.D. Sewall, and V.W. Lee. Implications of a metric for performance portability. Future Generation Computer Systems, 92:947 –958, 2019.

Evaluation Methodology

Interpreting and Visualising Performance Portability Metrics

- **A single portability metric may hide useful insights**
- **Analysis augmented with visualisations from Sewall et al. [2]**
- **Example (from [2])**
  - **Synthetic data set with 6 variants**
  - **Boxplots show median portability, spread and outliers**
  - **Cascade plots show how performance portability changes as platforms are added**



[2] J.D. Sewall, S.J. Pennycook, D. Jacobsen, T. Deakin, and S. McIntosh-Smith. Interpreting and visualizing performance portability metrics. In 2020 P3HPC Workshop, pages 14–24, 2020.

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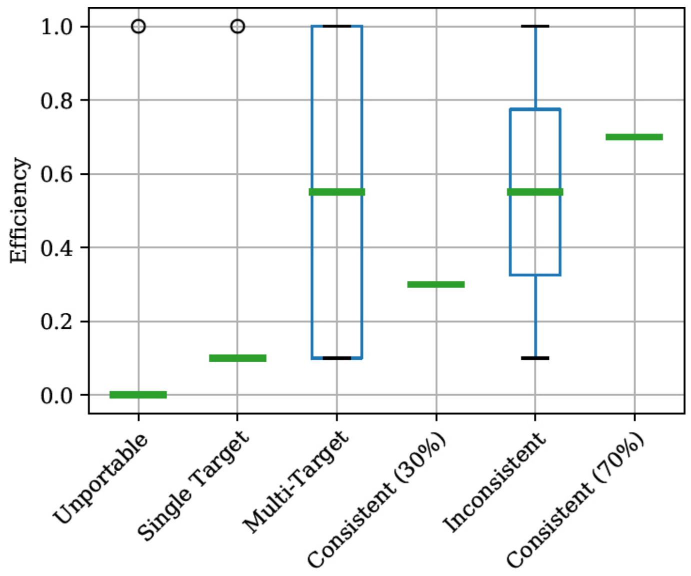

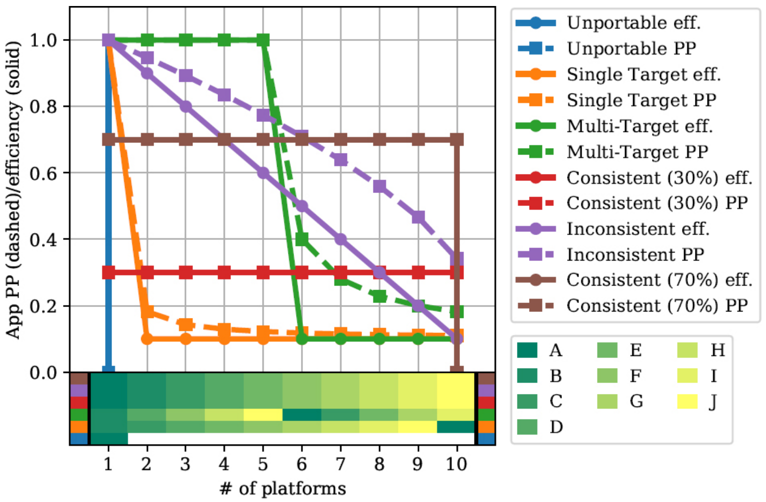

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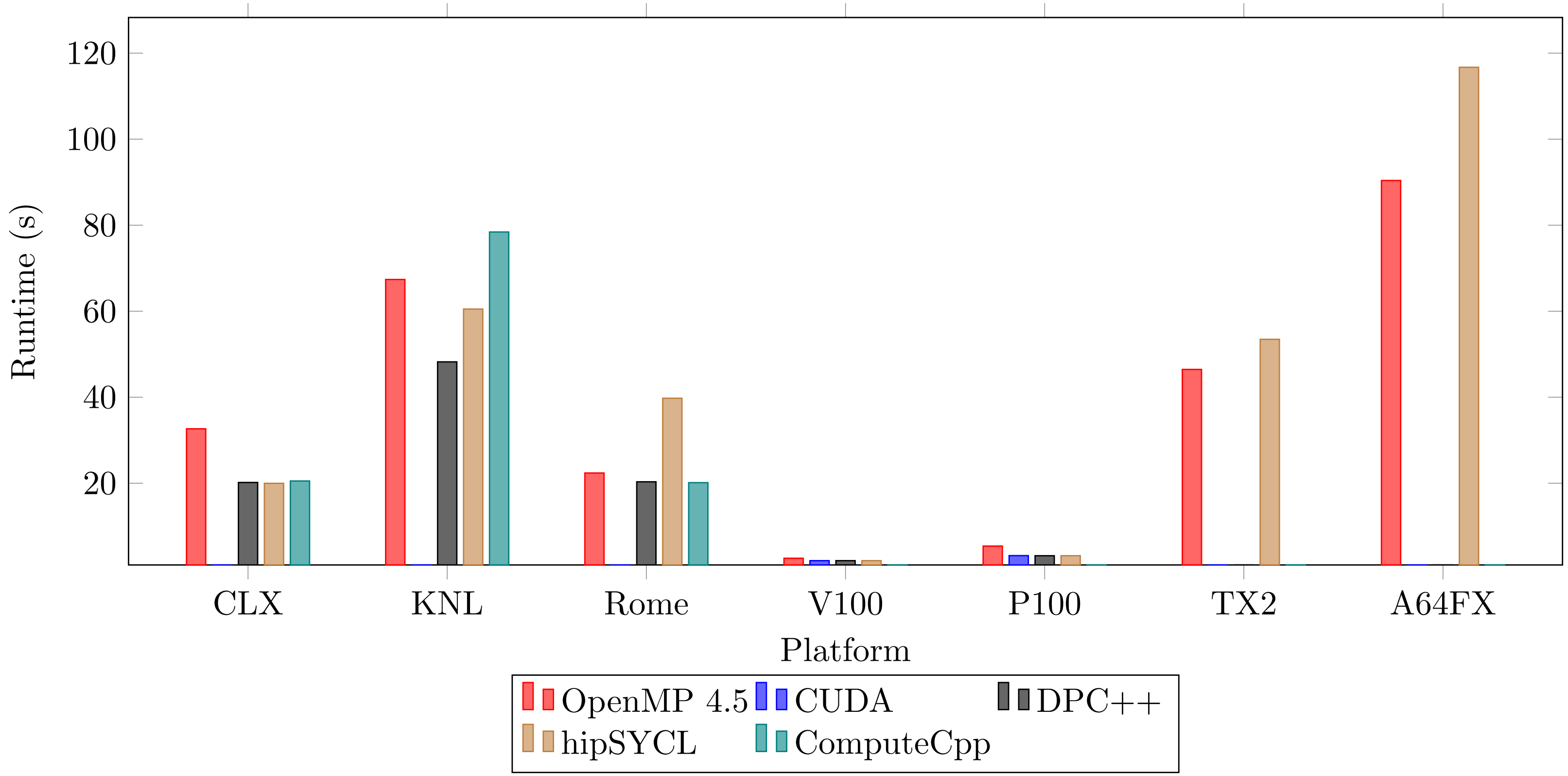
Evaluation of Approaches

Heat

- Simple finite difference heat equation on structured grid
- Results collected from Isambard



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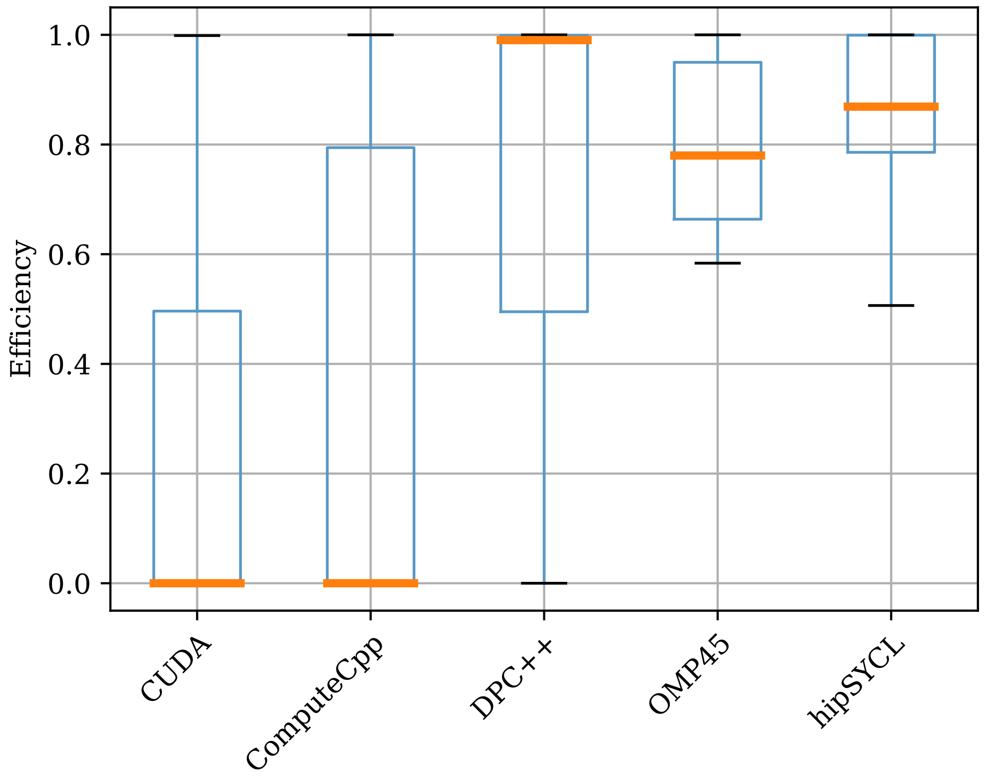

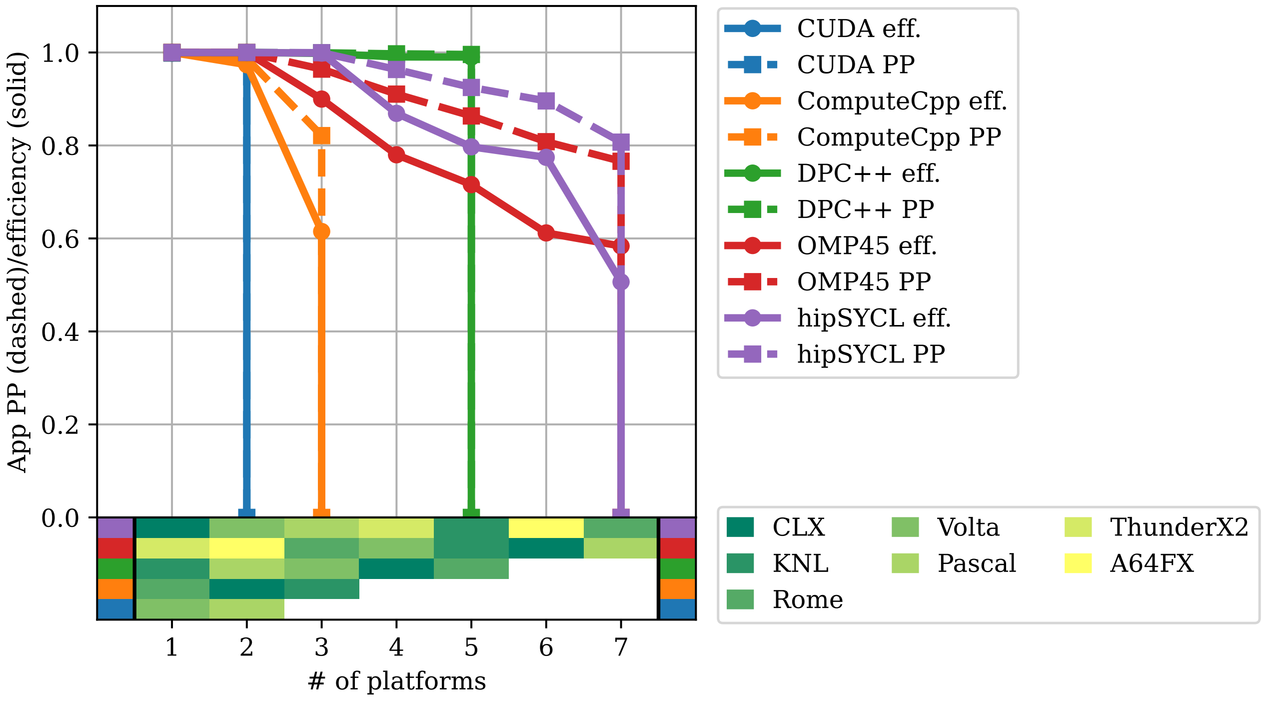

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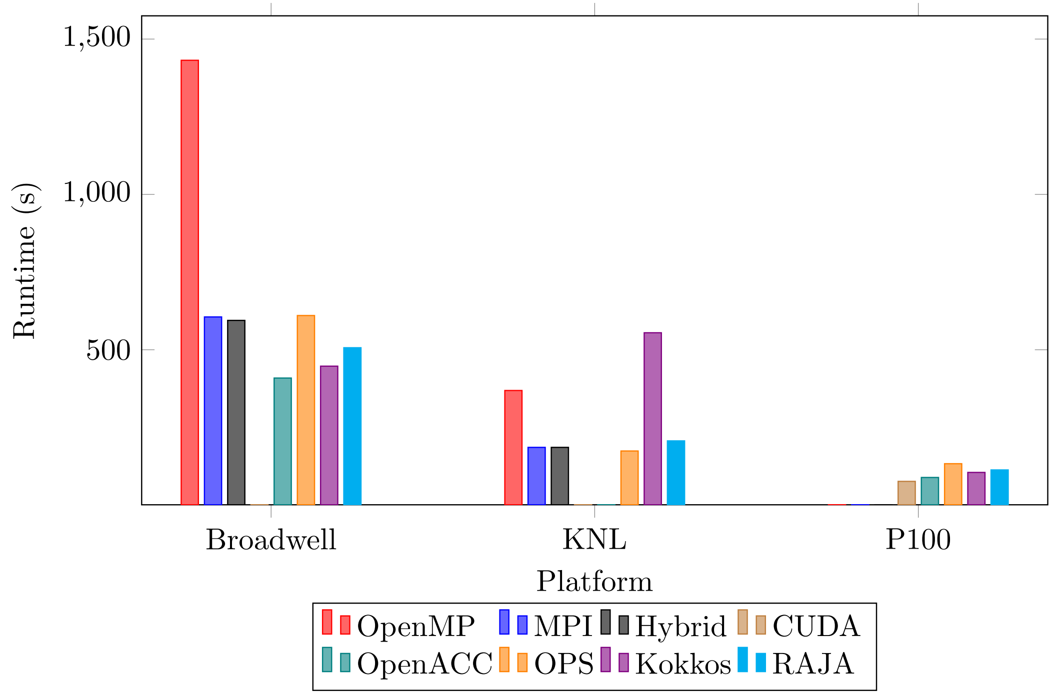
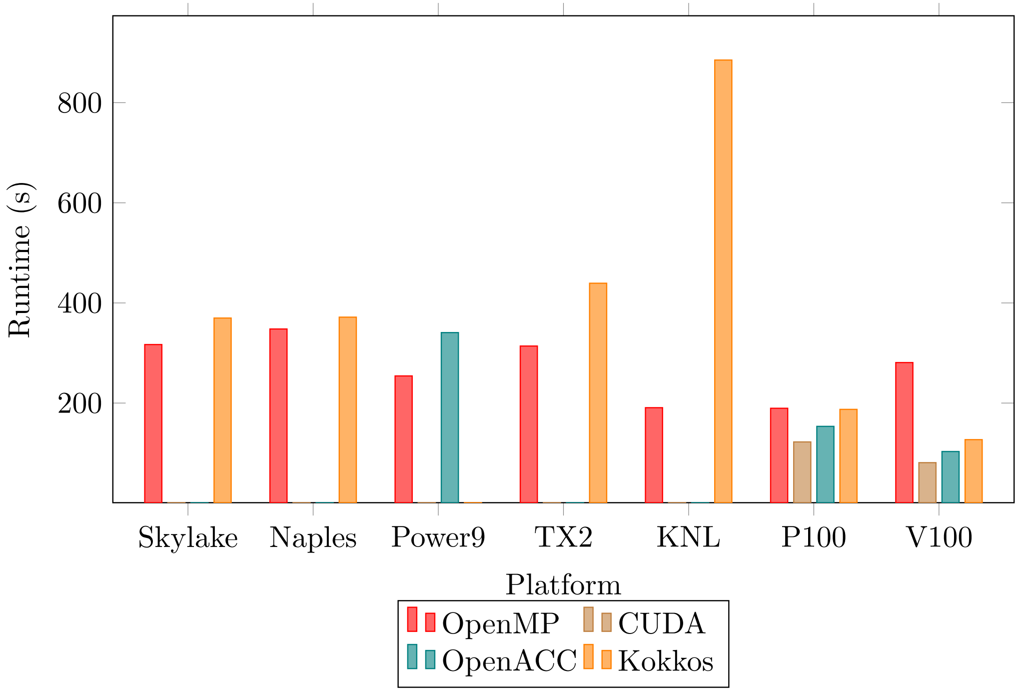
Evaluation of Approaches

TeaLeaf

- **Finite differencing on structured grid**
- **Performance data taken from two studies [3,4]**





[3] R. O. Kirk, G. R. Mudalige, I. Z. Reguly, S. A. Wright, M. J. Martineau, and S. A. Jarvis. Achieving Performance Portability for a Heat Conduction Solver Mini-Application on Modern Multi-core Systems. In IEEE CLUSTER, pages 834–841, Sep. 2017

[4] T. Deakin, S. McIntosh-Smith, J. Price, A. Poenaru, P. Atkinson, C. Popa, and J. Salmon. Performance portability across diverse computer architectures. In P3HPC Workshop, pages 1–13, 2019.

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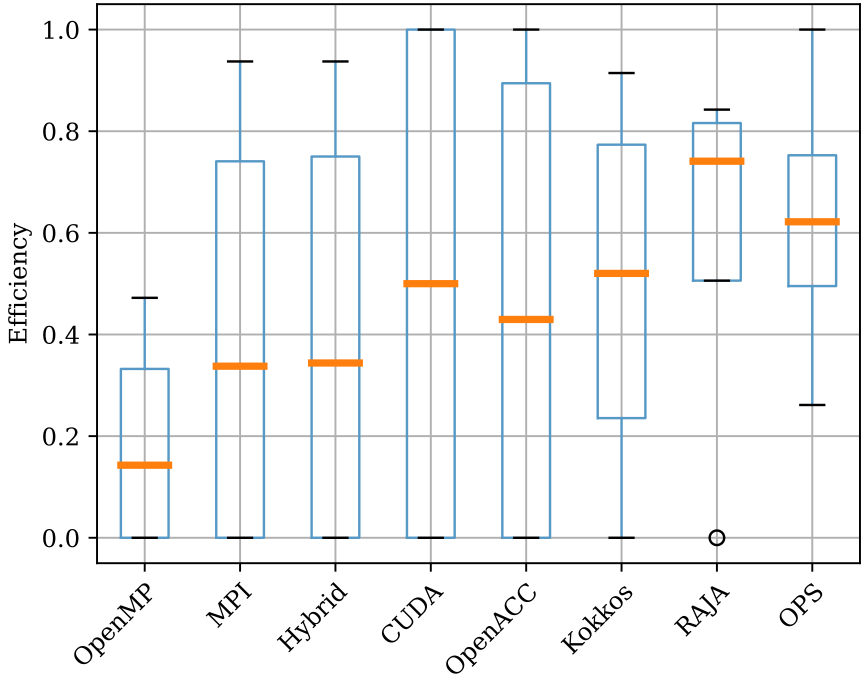

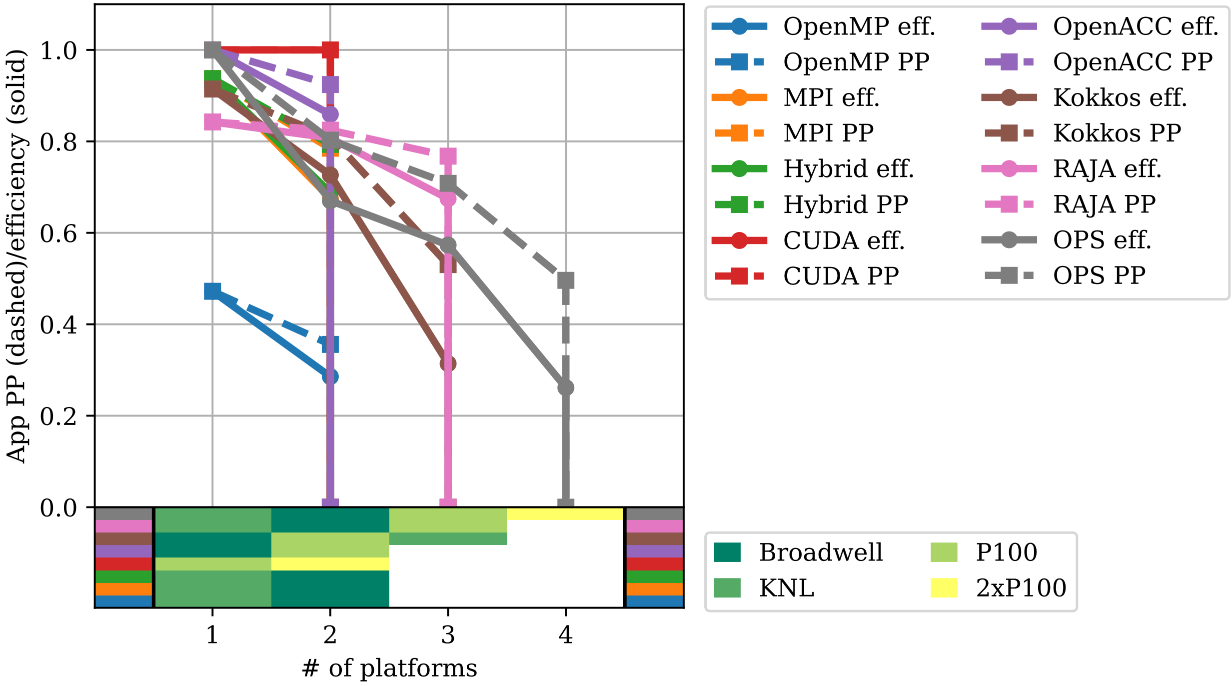

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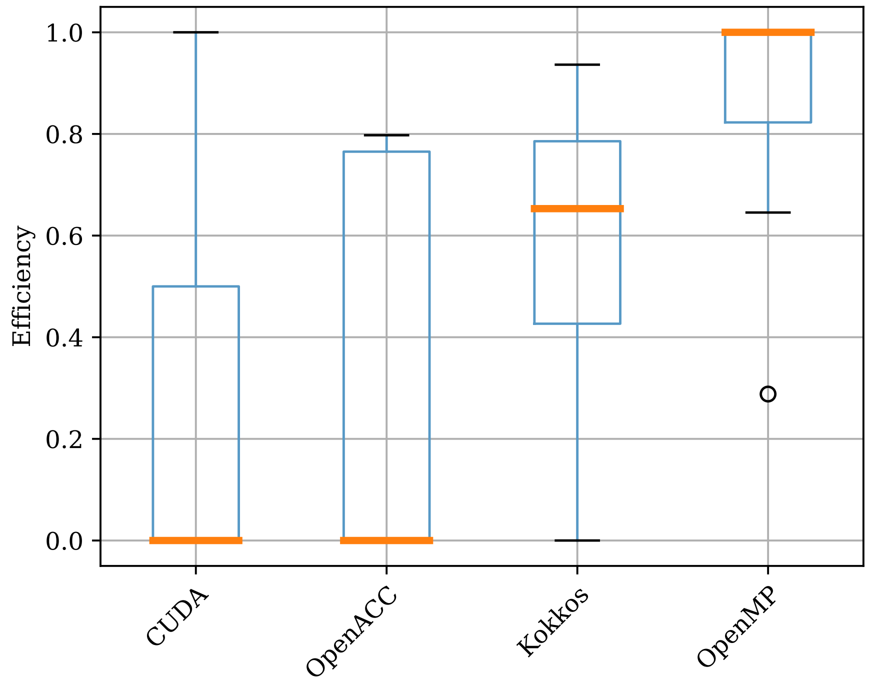

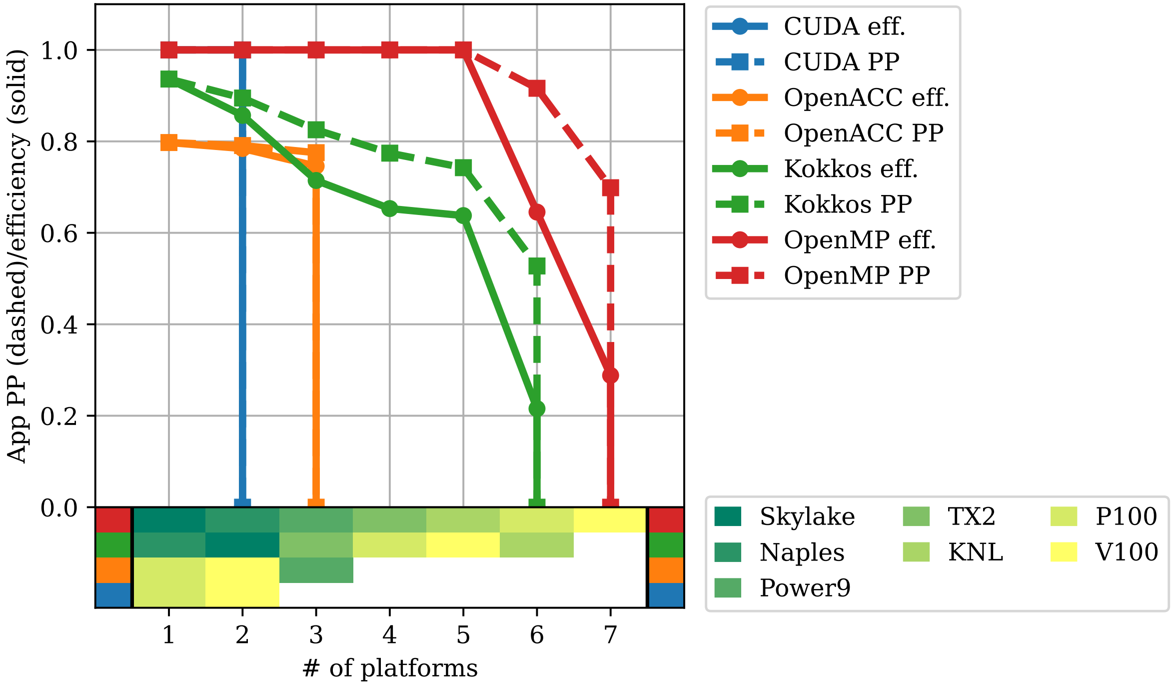

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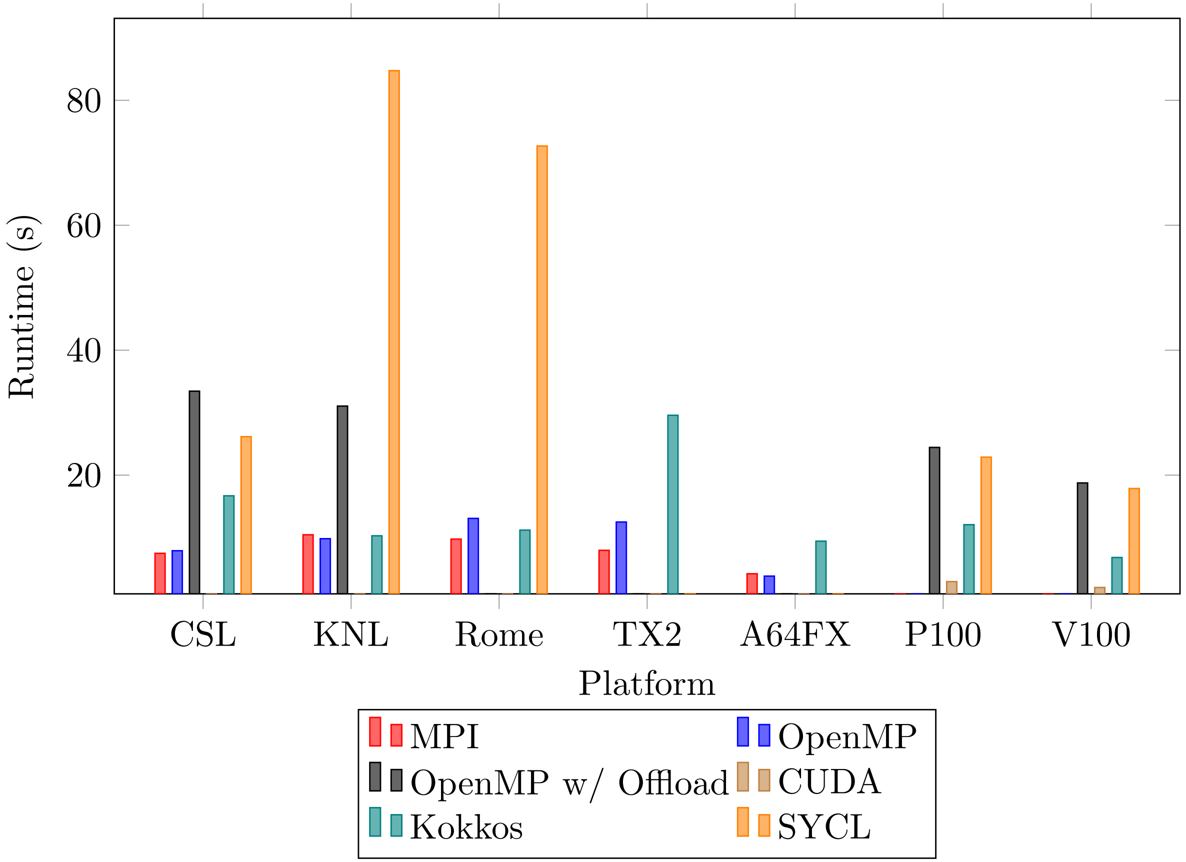
Evaluation of Approaches

miniFE

- **Finite element method code, part of Mantevo (now ECP Proxy Apps)**
- **Results collected from Isambard**



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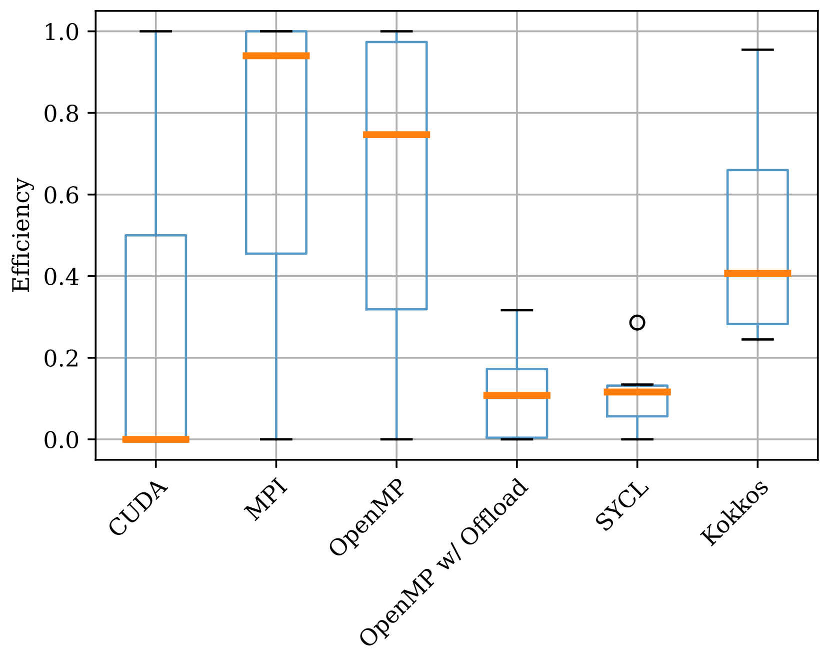
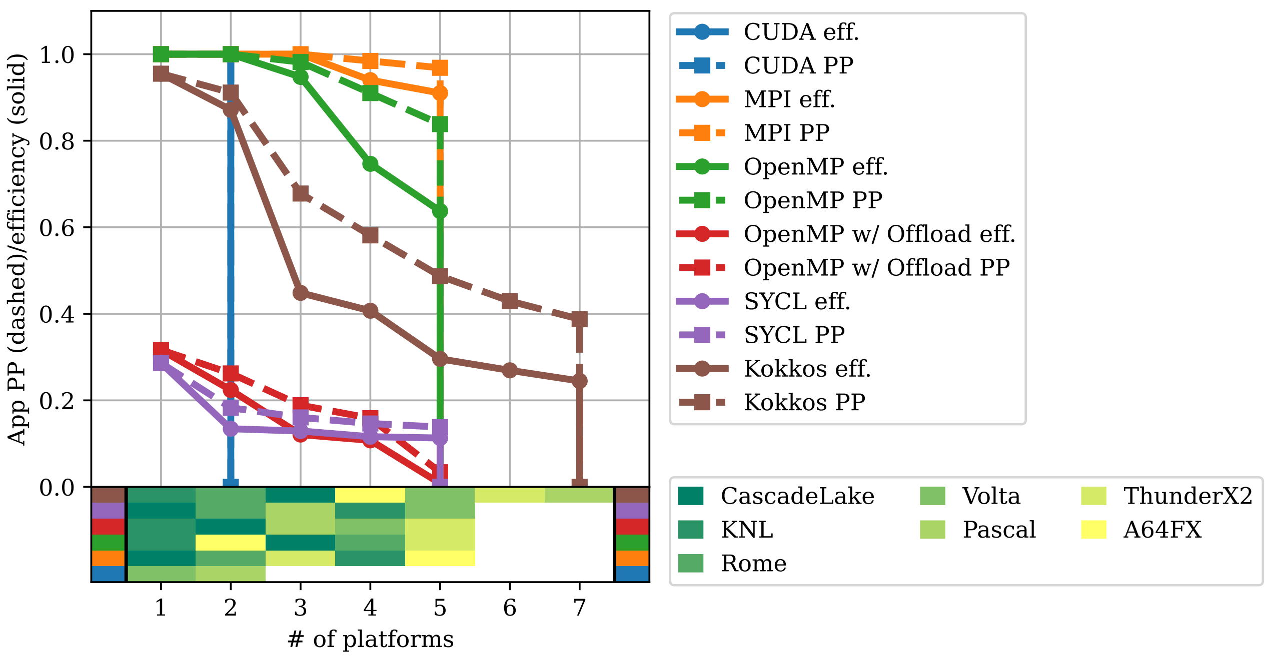
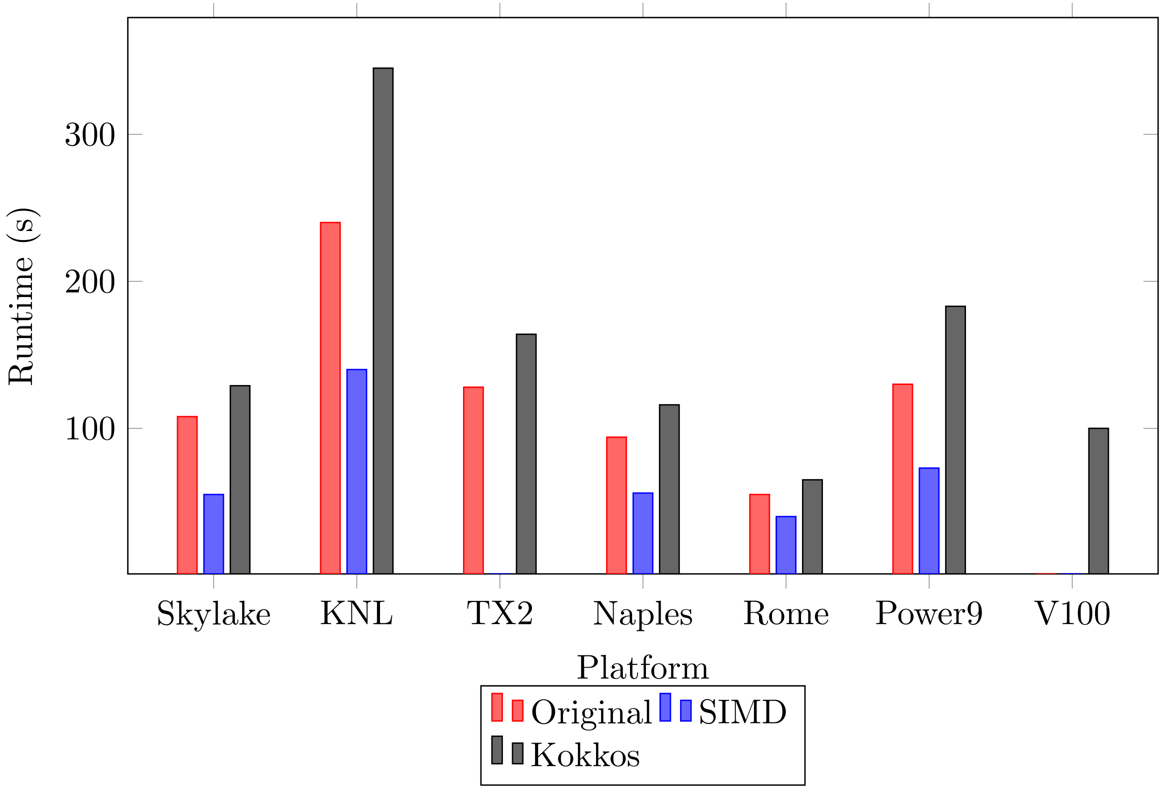




Evaluation of Approaches

VPIC/VPIC 2.0

- **Hand implemented vectorised kernels (native)**
- **VPIC 2.0 in Kokkos [5]**



[5] R. Bird, N. Tan, S.V. Luedtke, S. Harrell, M. Taufer, and B. Albright. VPIC 2.0: Next Generation Particle-in-Cell Simulations. IEEE Transactions on Parallel and Distributed Systems, pages 1–1,2021.

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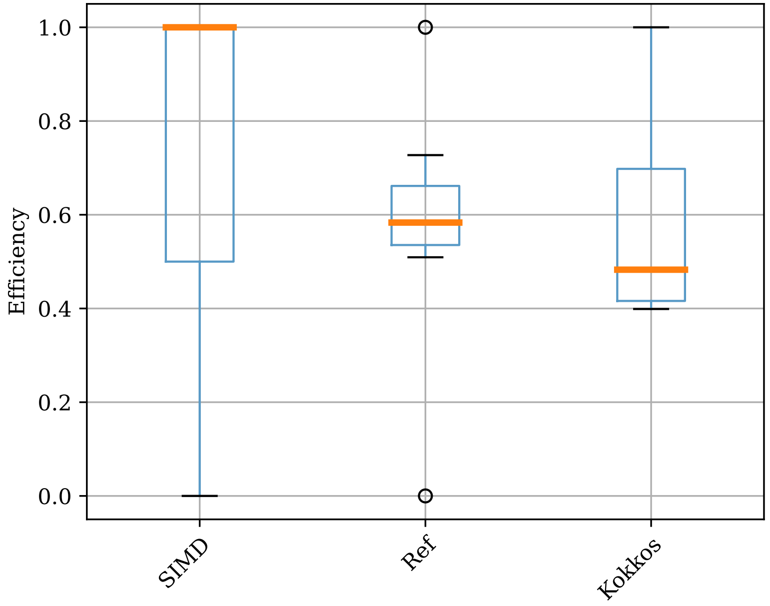

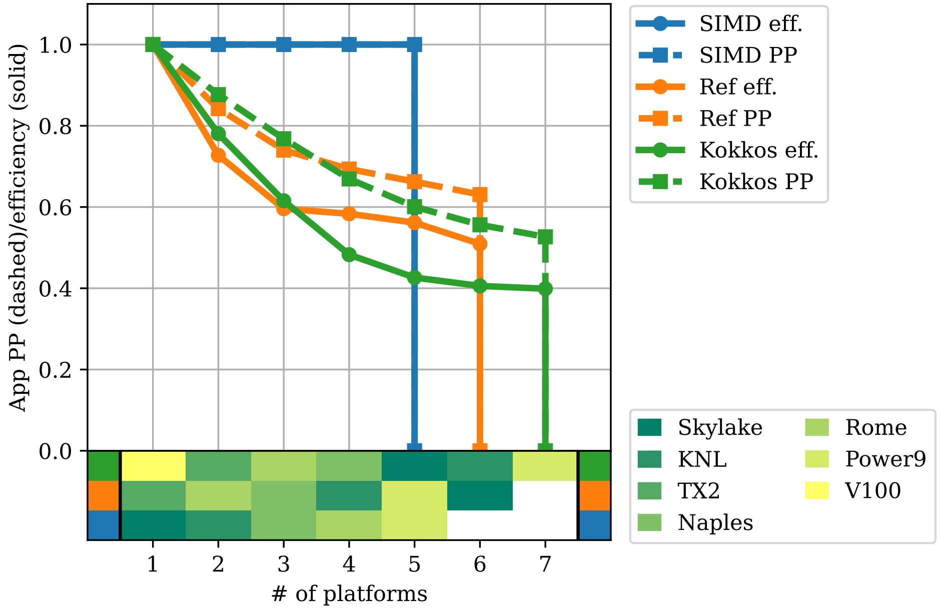

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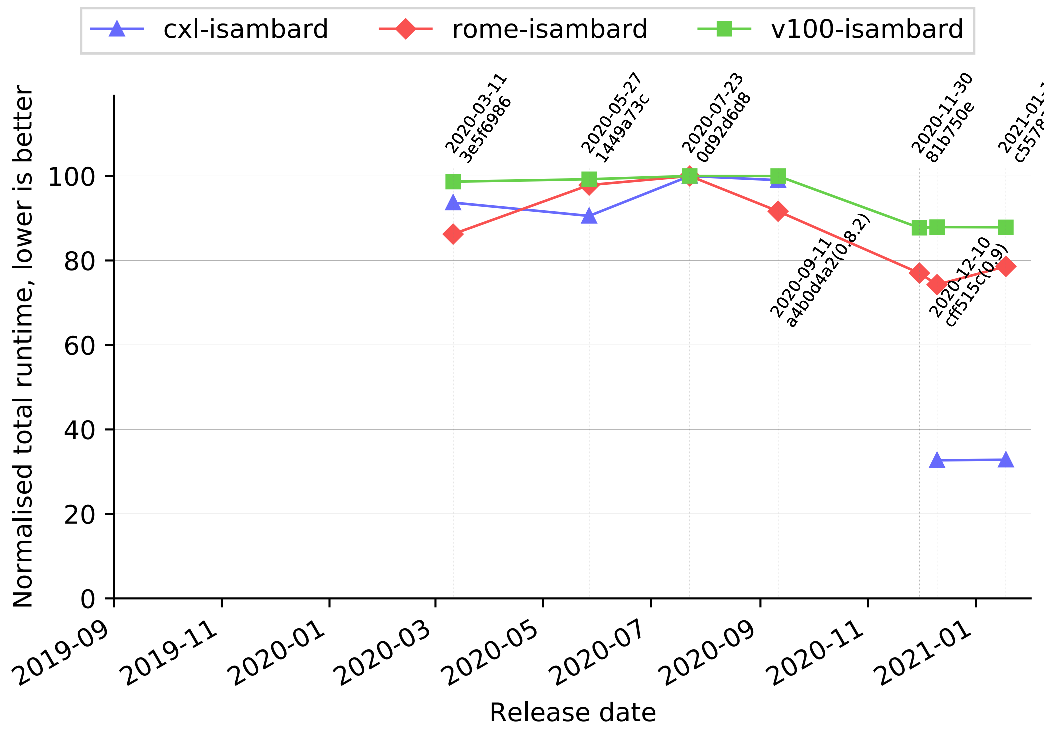
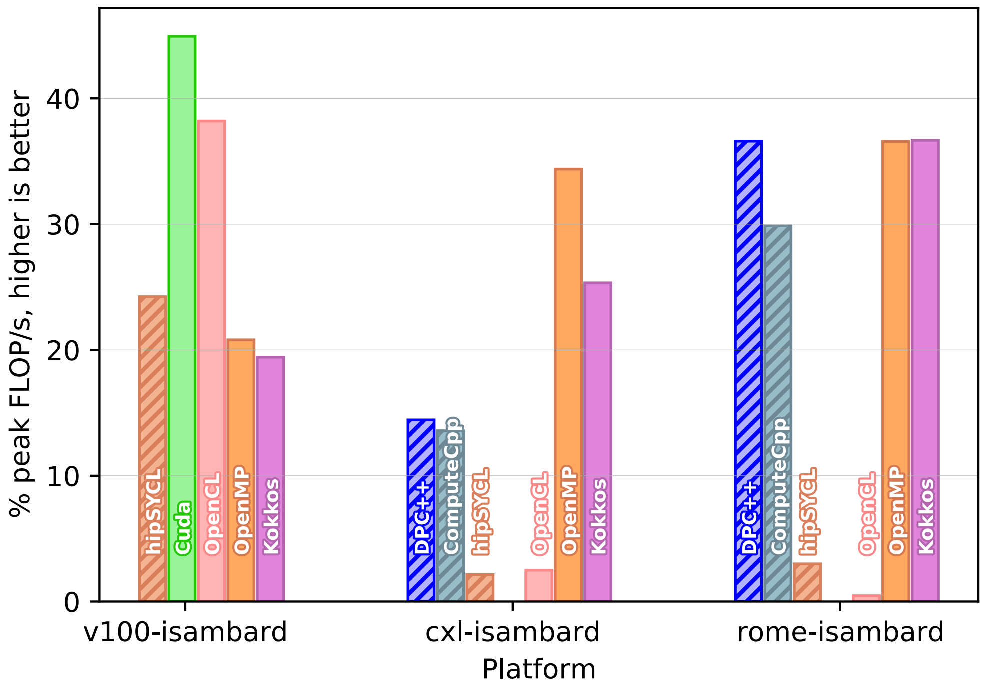
Evaluation of Approaches

Additional Results

- **Lin et al. have been tracking SYCL implementation maturity**
- **Evaluate BabelStream, BUDE and Cloverleaf**





[8] W.-C. Lin, T. Deakin, and S. McIntosh-Smith. On measuring the maturity of SYCL implementations by tracking historical performance improvements. In International Workshop on OpenCL, IWOCL'21, New York, NY, USA, 2021. ACM

ExCALIBUR

Evaluation of Approaches

Observations

- Pragma-based approaches (OpenMP, OpenACC)
  - Easiest to implement (or add) 👍
  - OpenMP can offer good portability across heterogeneous platforms 👍
  - … but really this requires different directives based on platform 👎
- Programming model approaches (Kokkos, RAJA, SYCL)
  - Kokkos and RAJA offer similar levels of performance portability 👍
  - SYCL evaluation currently limited, but we expect performance to improve with a change of compiler and compiler maturity 👍
- High-level DSL approaches (OPS, (py)OP2, UFL)
  - OPS/OP2 show good portability, but are parallel pattern based 👍

FM-WP4 Code Structure and Coordination

Support and Coordination

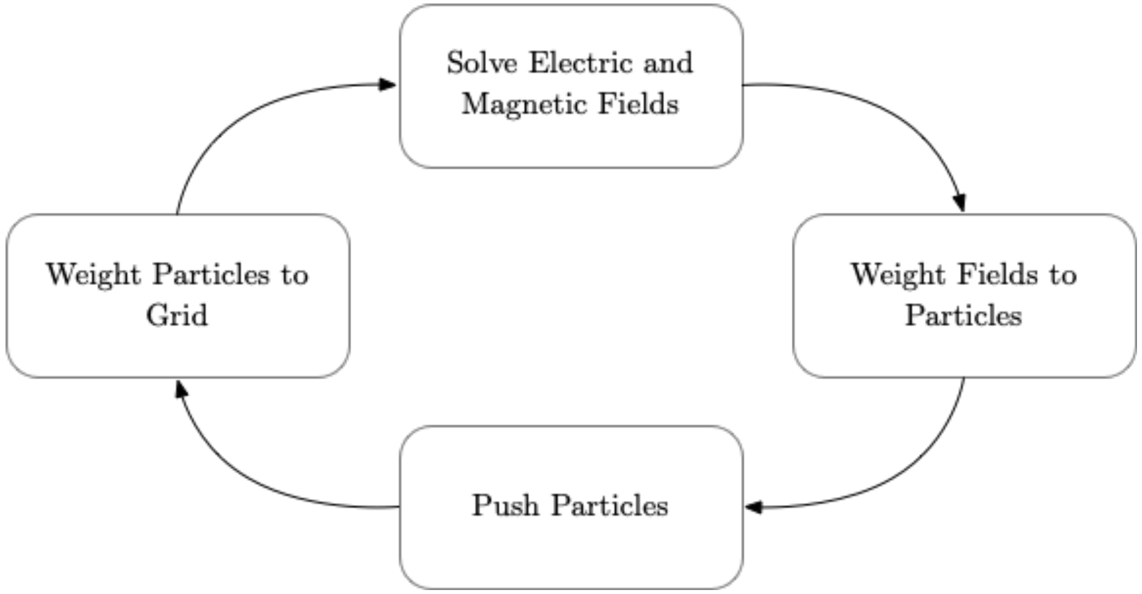
Our second project was also based around four deliverables:

- Periodic revision of Hardware and Software Reviews
- Development of an FEM-PIC mini-application
- Performance evaluation of FEM-PIC application
- Outline proposal for a particle-methods DSL

Developing an Unstructured PIC Mini-app

FEM-PIC

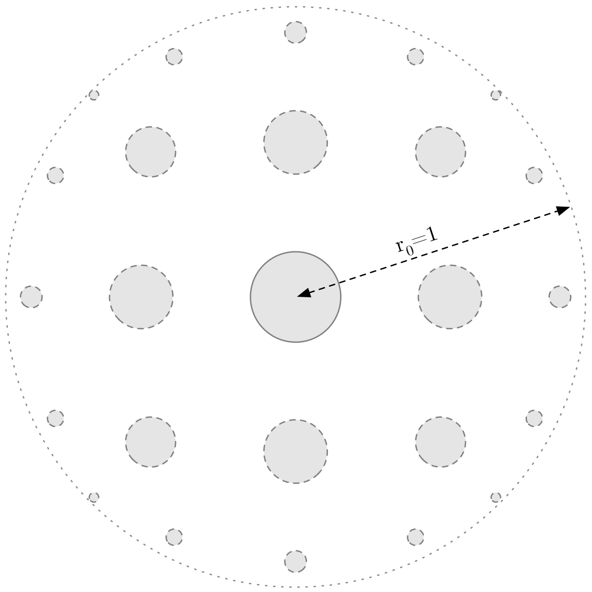
- Our evaluation has been limited to DoE PIC codes
  - All developed with Kokkos
  - All structured grid (except EMPIRE-PIC, but this is export controlled ☹️)
- Unstructured grid adds complexity that cannot easily be captured
  - Particle push necessitates a gather and scatter



Developing an Unstructured PIC Mini-app

FEM-PIC

```c
struct particle {
    double part_p[3];
    double part_pos[3];
    double weight;
    double charge;
    double mass;
    struct particle *next;
    struct particle *prev;
    int id;
};
```

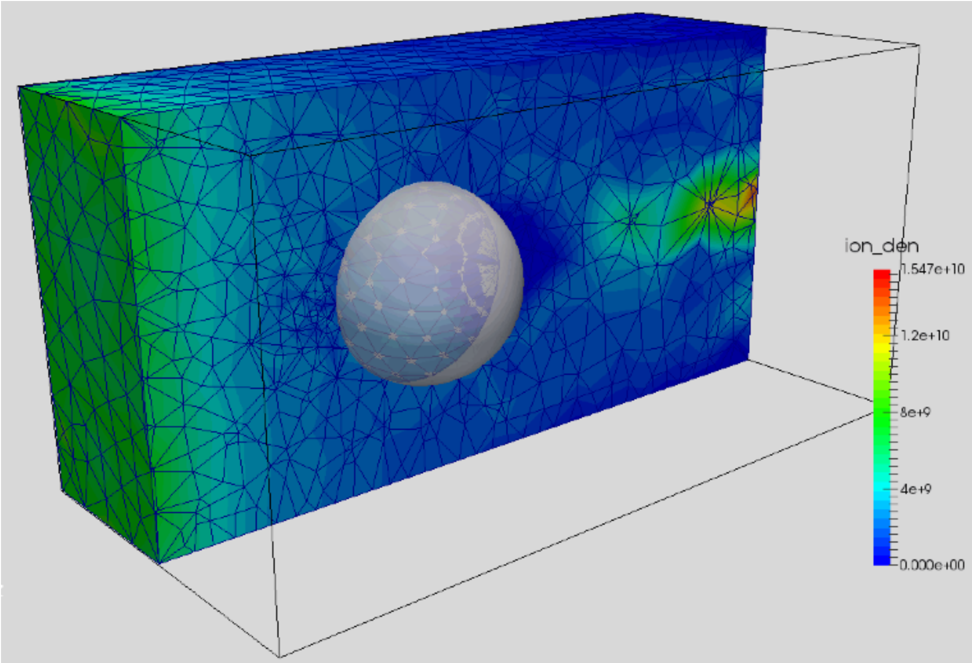


- **Goal is to add particles to an existing mini-application**
    - **Mimic storage used by EPOCH**
    - **Extract performance data from three key steps in particle movement**
- **~1000-3000 LOC**
    - **Enables rapid porting and evaluation**
    - **Enables analysis of novel storage techniques, particle shapes etc**

Developing an Unstructured PIC Mini-app

Progress

- Identified two candidate "base" applications
  - FEM implementation based on "Computational Physics" by Jos Thijssen
  - FEM-PIC from particleincell.com
- FEM-PIC likely the best candidate, but work needed to make it "look" more like EPOCH and EMPIRE



FM-WP4 Code Structure and Coordination

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Particle-methods DSL

Outline Proposal

- Many DSLs available for mesh-based codes
- Very few for particle-based codes
    - Notable examples include:
        - CoPA/Cabana — a library for data storage and manipulation of particle data
        - HartreeParticleDSL — Particle methods DSL, using Regent programming language
        - PPMD — Particle DSL mainly for particle-particle interactions (e.g. molecular dynamics)

Particle-methods DSL

Outline Proposal

- **Need for a Particle DSL that can interact with a Mesh DSL**
- **Following development of FEM-PIC mini-application:**
  - **Field solver will be redeveloped using OP2**
  - **Sketch out requirements for a DSL for particles**
  - **Proposal of an API**

PROJECT NEPTUNE

WORK PACKAGE 4: SUPPORT AND COORDINATION

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