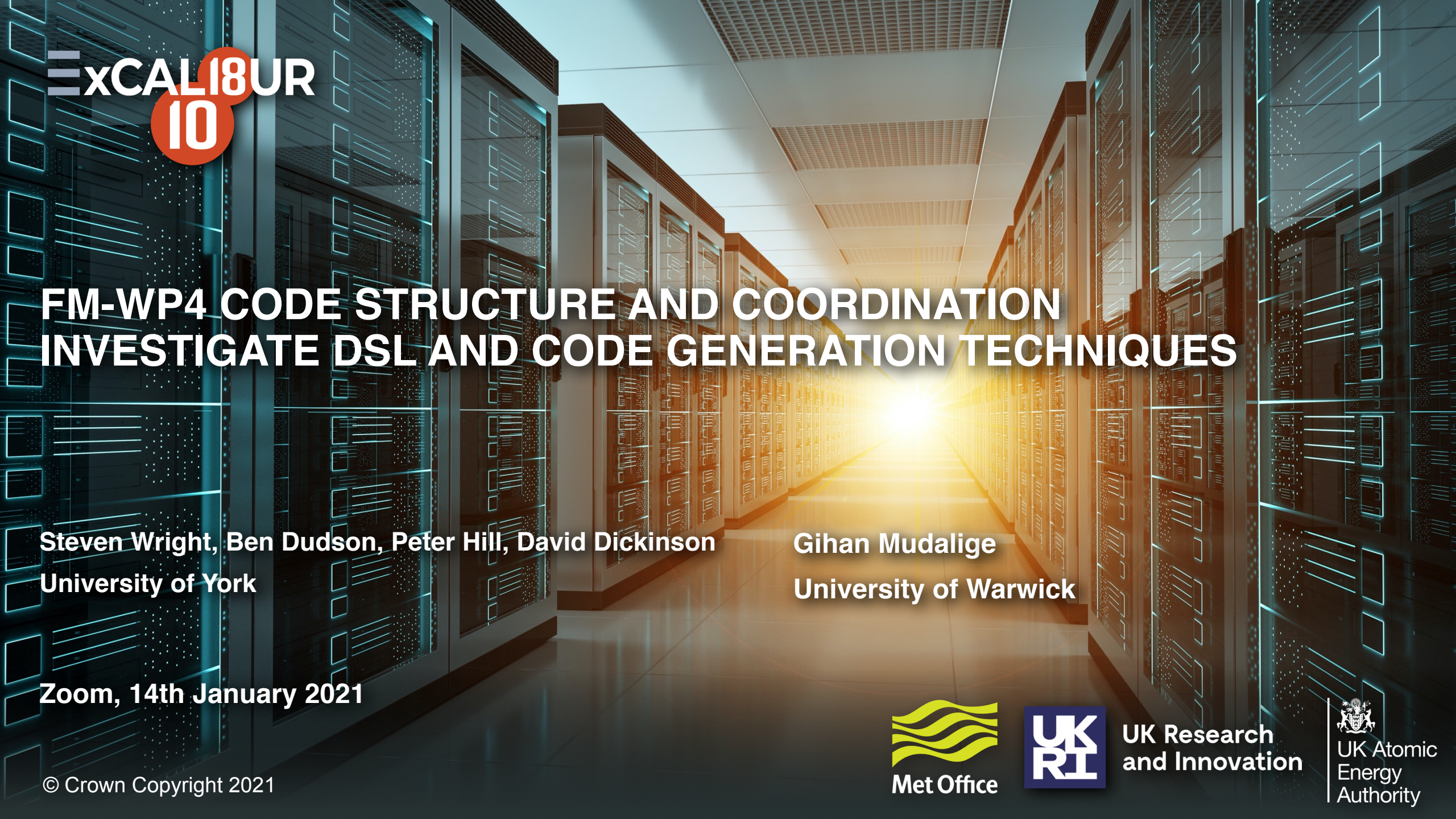

# FM-WP4 CODE STRUCTURE AND COORDINATION INVESTIGATE DSL AND CODE GENERATION TECHNIQUES


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Zoom, 14th January 2021

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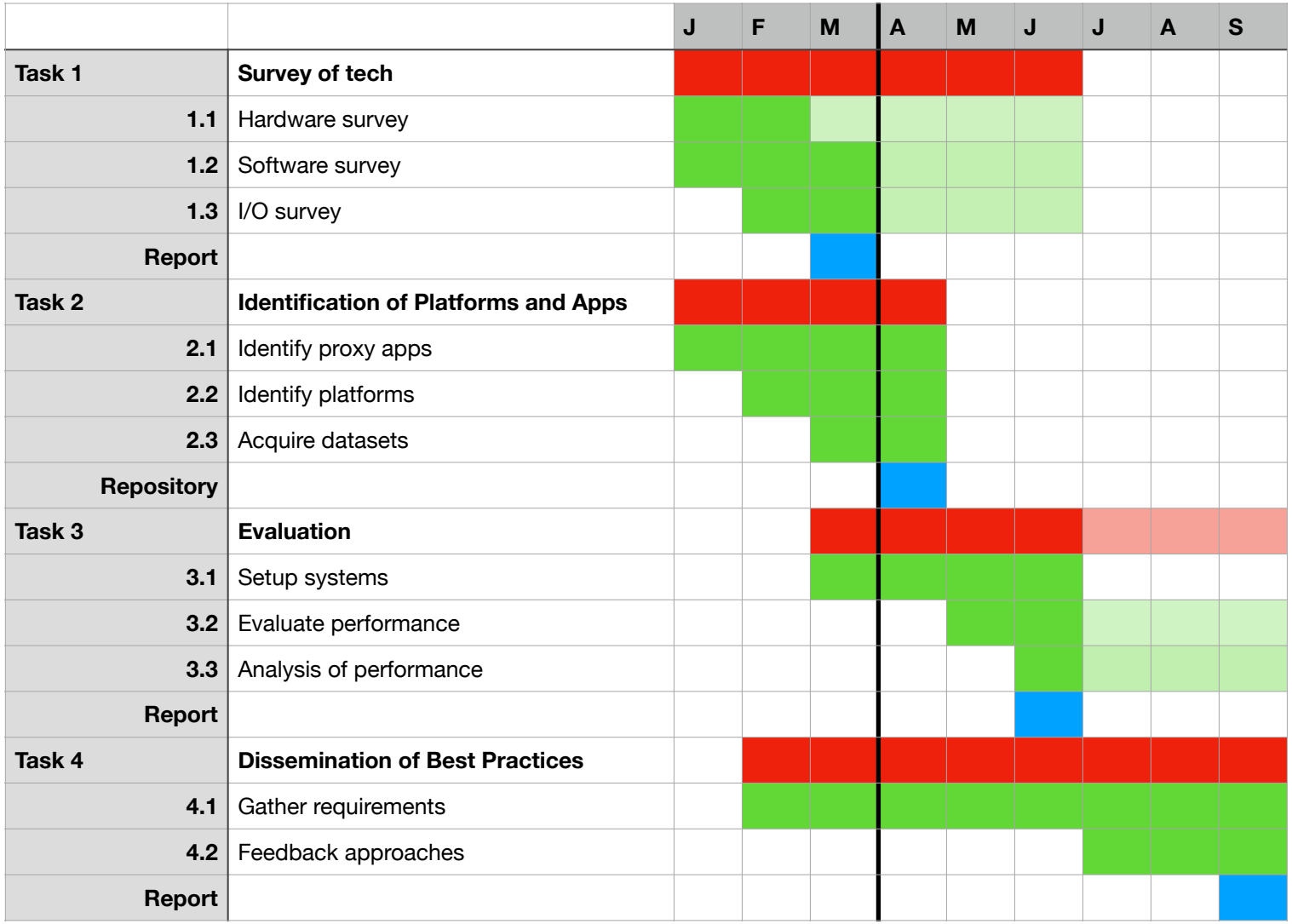
# Project Timeline

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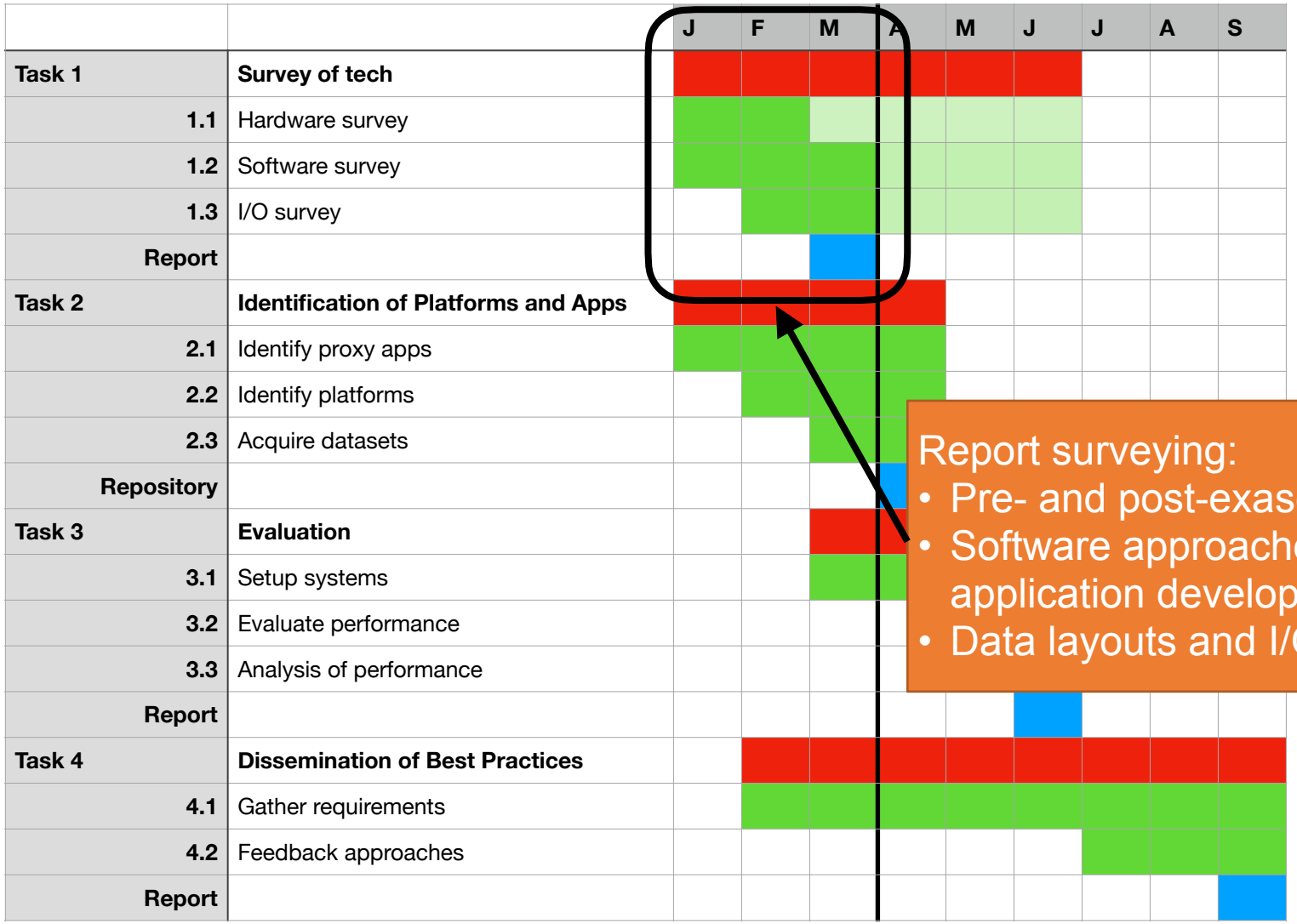
# Task 1

## Survey of available technology




Report surveying:

- Pre- and post-exascale hardware
- Software approaches to Exascale application development
- Data layouts and I/O

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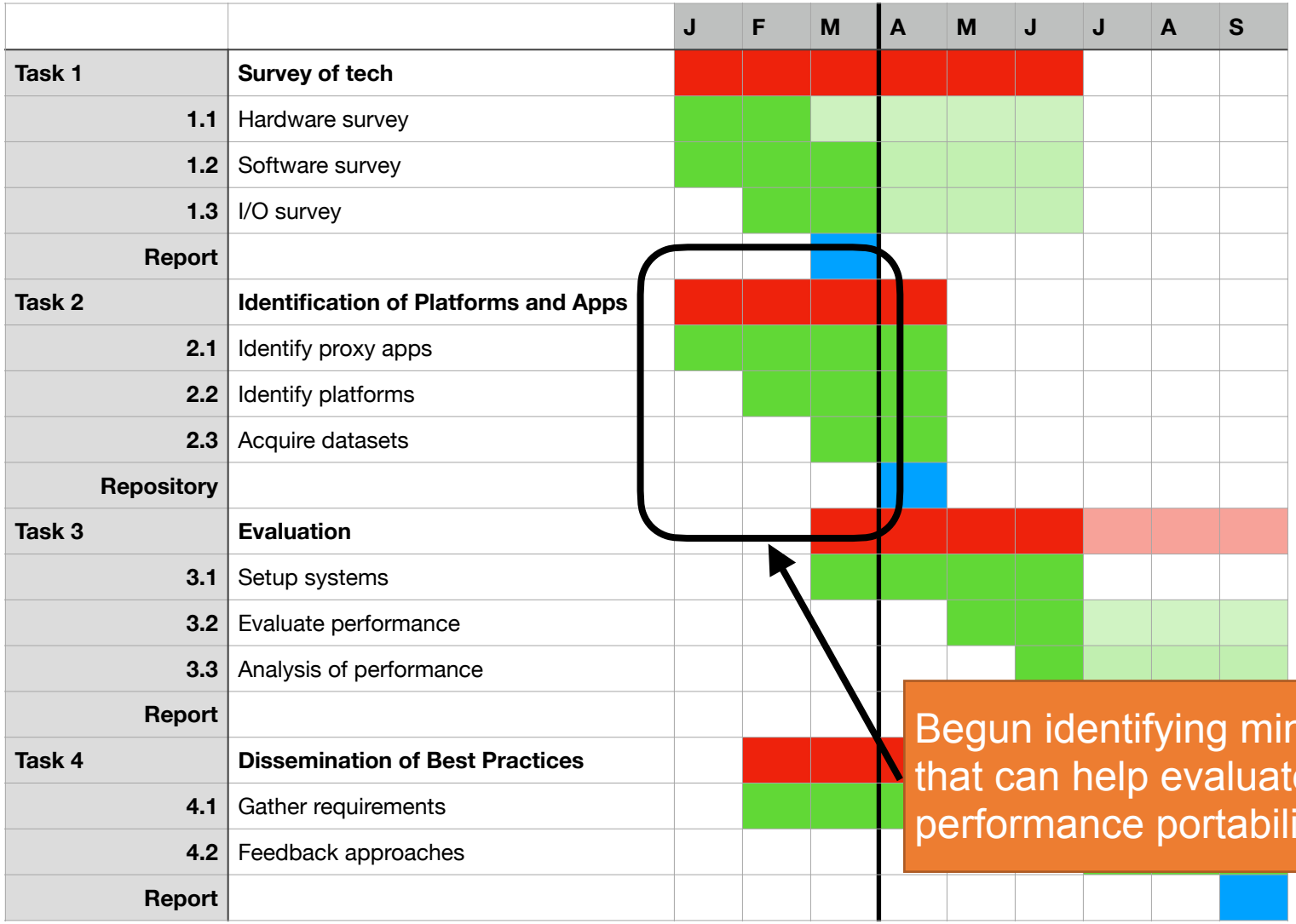
# Task 2

## Identification of Platforms and Applications




Begun identifying mini-apps/proxy-apps that can help evaluate approaches to performance portability.

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# Task 1.1

## 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 (Lovelace/Hopper/Einstein?)
  - AMD Instinct
  - Intel Xe
- Most systems will use x86_64 hosts from Intel and AMD


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# Task 1.1

## Pre- and Post-Exascale Hardware


DoE have 4 Cray Shasta systems in the pipeline

- All Cray Shasta Systems with Slingshot Fabric
- Perlmutter
  - >100 PFLOP/s
  - AMD EPYC CPUs with NVIDIA A100 GPUs
- Aurora
  - 1 EFLOP
  - Intel Xeon CPUs (Sapphire Rapids) with Intel Xe GPUs
- Frontier
  - 1.5 EFLOP/s
  - AMD EPYC CPUs (Milan) with AMD Instinct GPUs
- El Capitan
  - 2 EFLOP/s
  - AMD EPYC CPUs (Genoa) with AMD Instinct GPUs

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# Task 1.1

## Pre- and Post-Exascale Hardware

**Europe has 3 pre-Exascale systems in development**

- **LUMI**
  - **0.5 EFLOP/s**
  - **AMD EPYC CPUs with AMD Instinct GPUs**
- **LEONARDO**
  - **0.3 EFLOP/s**
  - **Intel Xeon CPUs (Sapphire Rapids) with NVIDIA A100 GPUs**
- **MareNostrum 5**
  - **2 distinct 100+ PFLOP/s systems**
  - **Unknown architectures, but possible use of ARM/RISC-V**

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# Task 1.1

## Pre- and Post-Exascale Hardware

In the UK,

- ARCHER-2
  - ~28 PFLOP/s
  - AMD EPYC CPUs
  - Cray Slingshot Fabric
- Many Tier-2 systems
  - Isambard-2
    - A64FX, AMD EPYC, NVIDIA GPUs, AMD GPUs, etc
  - Bede, Viking, Avon, etc

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# Task 1.1

## Software Approaches to Exascale

- Hardware is diversifying rapidly…
- Portable software more important than ever before!
- Many approaches,
  - OpenMP/OpenACC directive-based methods
  - OneAPI/SYCL/OpenCL programming models
  - Kokkos/RAJA-style template libraries
  - PETSc/BLAS-style kernel libraries
  - OP2/OPS-style domain specific languages


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# Task 1.1

## Software Approaches to Exascale

- Some Domain Specific Languages are low-level APIs aimed at developers
  - e.g. OP2 is a programming abstraction for unstructured mesh algorithms
- Some are high-level, aimed at allowing scientists to express the equations they're trying to solve
  - e.g. UFL, BOUT++

```
//main time-marching loop
for(int iter=1; iter<=niter; iter++) {
    // save old flow solution
    op_par_loop(save_soln, ... );

    // predictor/corrector update loop
    for(int k=0; k<2; k++) {

      // calculate area/timstep
      op_par_loop(adt_calc, ... );

      // calculate flux residual
      op_par_loop(res_calc, ... );
```

$$\frac{\partial \rho}{\partial t} = -\mathbf{v} \cdot \nabla \rho - \rho \nabla \cdot \mathbf{v}$$
$$\frac{\partial p}{\partial t} = -\mathbf{v} \cdot \nabla p - \gamma p \nabla \cdot \mathbf{v}$$
$$\frac{\partial \mathbf{v}}{\partial t} = -\mathbf{v} \cdot \nabla \mathbf{v} + \frac{1}{\rho}(-\nabla p + (\nabla \times \mathbf{B}) \times \mathbf{B})$$
$$\frac{\partial \mathbf{B}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B})$$

can be written simply as:

```
ddt(rho) = -V_dot_Grad(v, rho) - rho*Div(v);
ddt(p)   = -V_dot_Grad(v, p) - g*p*Div(v);
ddt(v)   = -V_dot_Grad(v, v) + (cross(Curl(B),B) - Grad(p))/rho;
ddt(B)   = Curl(cross(v,B));
```

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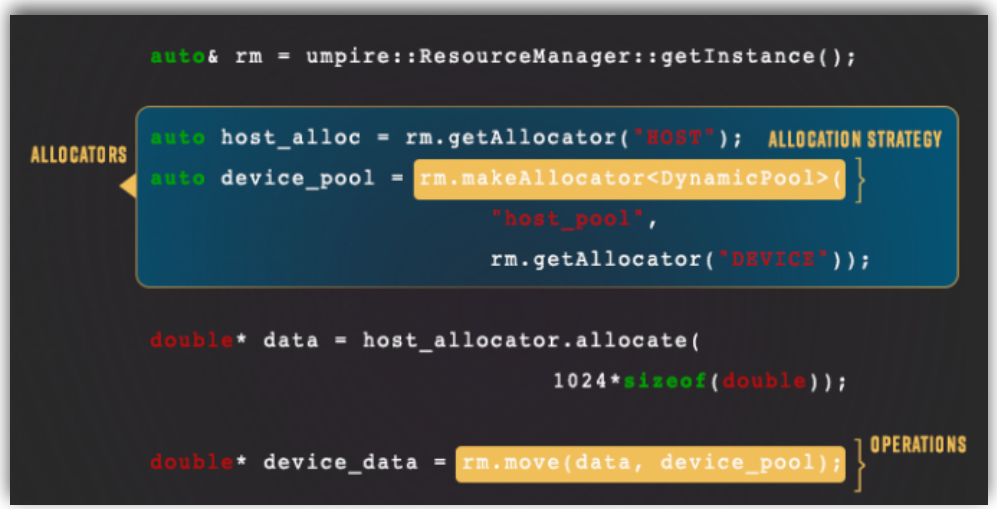
# Task 1.1

## Data representation and I/O

```
// A Default 3D-View with 2 runtime dimensions.
// This View will be reference counted
Kokkos::View<double**[8]> A(?A-Default?,1000,256);

// An atomic view of A. Every access (=,+=,=-,?) will be atomic.
// This View will be reference counted (i.e. it has a shared reference count with A
Kokkos::View<double**[8], Kokkos::MemoryTraits<Kokkos::Atomic> A-Atomic = A;
```




- With hierarchical parallelism, optimised data representation and movement are vital
  - Managing data transparently to the user
    - Kokkos Views
    - UMPIRE
    - Intel SDLT
  - API access that can be optimised for host architectures to ensure coalesced or strided accesses (where appropriate)

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# Task 1.1

## Data representation and I/O

- I/O improvements typically lag compute improvements
- Standardised output format libraries
  - HDF5, netCDF
- Libraries for accelerated I/O
  - TyphonIO, SILO, ADIOS

- New approaches are emerging: e.g. NVMe, VeloC, Rabbit

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# Task 1.1

## Conclusions

- Rewriting legacy codes for new heterogenous architectures 👎
- NEPTUNE is an opportunity to prepare a future-proofed code
- Important that we:
  - choose a programming model or DSL that supports many (or all!) backends 👍
  - choose an approach to data management that is hardware agnostic 👍
  - choose a user-interface (or DSL) that allows scientists to express problems without being overly restrictive 👍

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# Task 2

## Identification of testbed platforms and representative proxy applications

- NEPTUNE will require some coupling between Fluid and Particle models
- BOUT++/Nektar/EPOCH/Firedrake are likely too large to evaluate for portability
- A number of mini-applications exist in a variety of performance portable implementations (or are simple enough that they can be ported) that we can leverage to evaluate these approaches
  - FEM/Spectral
    - MiniFE, Nekbone
  - PIC
    - MinEPOCH, VPIC, PICSARlite
  - Suggestions on a postcard…

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