

# PROJECT NEPTUNE

## WORK PACKAGE 4: SUPPORT AND COORDINATION

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# FM-WP4 Code Structure and Coordination

## Software Support Procurement

**Based around three deliverables:**

- **Continual monitoring and update of state-of-the-art reviews**
- **Demonstrator implementations**
- **Edge Physics consultancy**

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# FM-WP4 Code Structure and Coordination

## Software Support Procurement

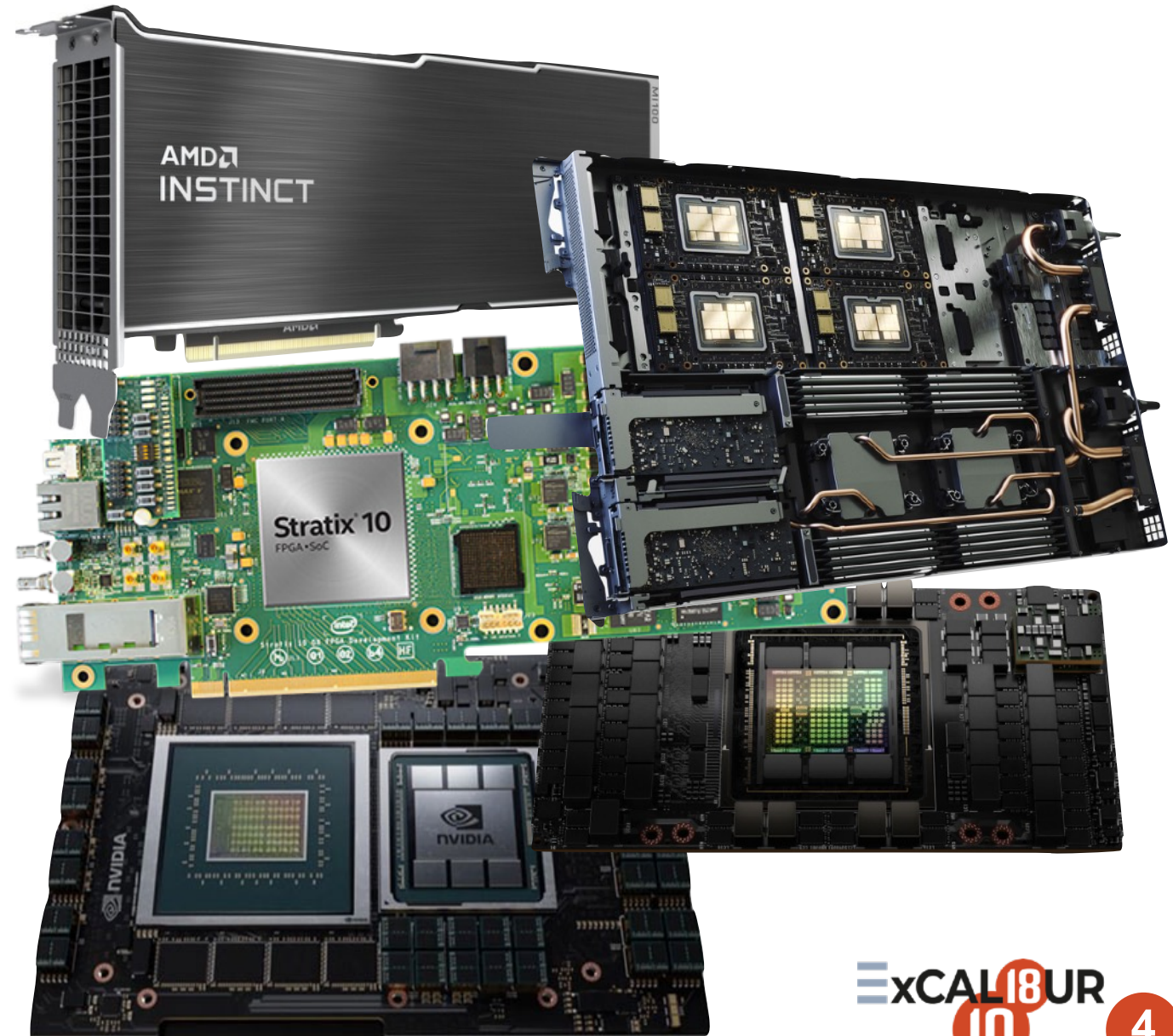
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# State-of-the-art Reviews

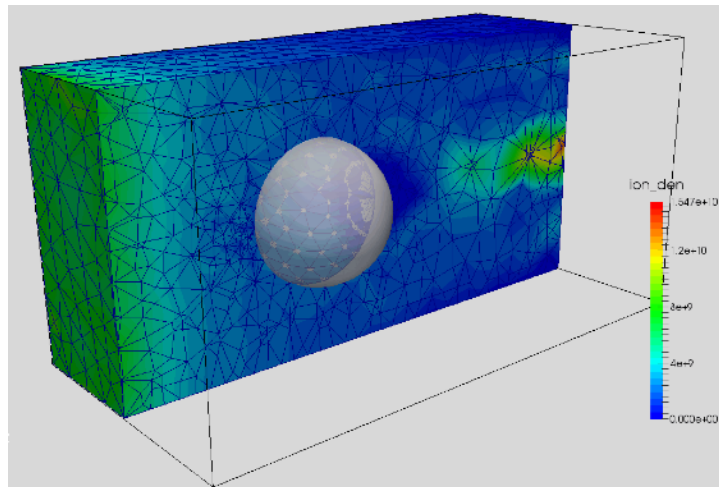
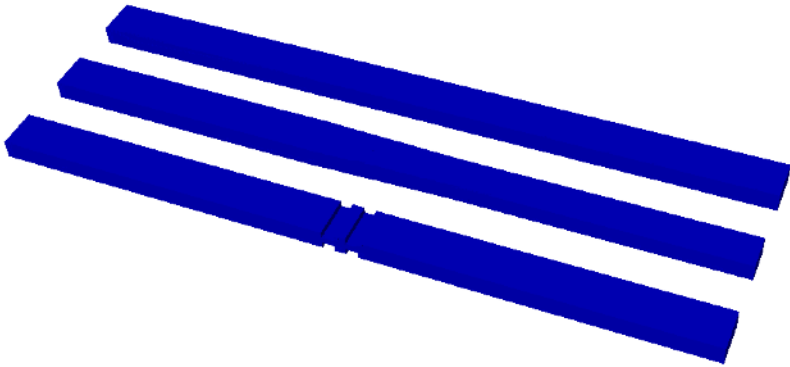
## New Hardware

- Evaluate new hardware (assuming access)
  - **AMD** GPUs (and new CPUs)
  - **Intel** GPUs (... and new CPUs)
  - **AMD/Intel** FPGAs
  - **NVIDIA** GPUs and CPUs
  - ...?



# State-of-the-art Reviews

## New Applications



- **Fluid Codes**

- FDTD3D – 3D Maxwell solver on fixed grid using Yee method
- MAXWELL – Maxwell FEM code implemented in MFEM
- HIPBONE – GPU port of Nekbone spectral element code

- **Particle Codes**

- SHEATH-PIC – 1D PIC code with GPU implementations
- FEM-PIC – Our developed PIC mini-app

- Assess representativeness (e.g. cosine similarity)

# State-of-the-art Reviews

## New Programming Models

- Increase coverage of programming models
  - More SYCL evaluations
  - Evaluation with different SYCL compilers
  - Julia
  - More OP-DSL evaluations
  - ... etc
- Maintain and expand our evaluation repository



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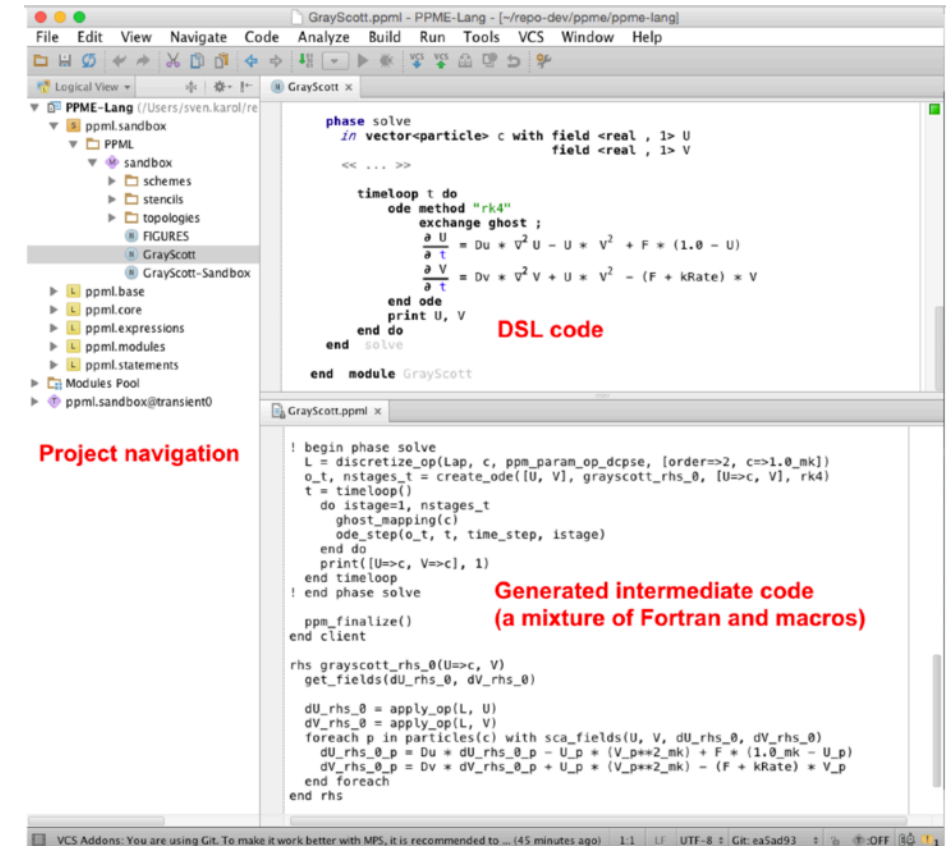
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# Demonstrator Applications

## Mini-applications as DSL Demonstrators

- T/AW087/21 will culminate in a proposal for a particle-based DSL
- This project will rely on collaboration with UKAEA, consulting on development of a new DSL for hybrid fluid/particle simulations



The screenshot displays the PPME-Lang IDE interface. On the left, a 'Project navigation' pane shows a tree structure of the project, including folders like 'ppml.sandbox', 'PPML', 'sandbox', 'schemes', 'stencils', 'topologies', 'FIGURES', 'GrayScott', and 'GrayScott-Sandbox'. The main editor area is split into two panes. The top pane, titled 'GrayScott.x', contains DSL code for a GrayScott simulation, including a 'phase solve' block with a 'timeloop' and 'ode method' for 'rk4'. The bottom pane, titled 'GrayScott.ppmi.x', shows the 'Generated intermediate code (a mixture of Fortran and macros)', which is a more detailed Fortran-like implementation of the same simulation logic. Red text labels 'DSL code' and 'Generated intermediate code (a mixture of Fortran and macros)' are overlaid on their respective code blocks.

```
phase solve
in vector<particle> c with field <real, 1> U
                        field <real, 1> V

<< ... >>

timeloop t do
  ode method "rk4"
  exchange ghost ;
  dU/dt = Du * V^2 U - U * V^2 + F * (1.0 - U)
  dV/dt = Dv * V^2 V + U * V^2 - (F + kRate) * V
end ode
print U, V
end do
end solve

end module GrayScott
```

```
! begin phase solve
L = discretize_op(Lap, c, ppm_param_op_dcpse, [order=>2, c=>1.0_mk])
o_t, nstages_t = create_ode([U, V], grayscott_rhs_0, [U=>c, V], rk4)
t = timeloop()
do istage=1, nstages_t
  ghost_mapping(c)
  ode_step(o_t, t, time_step, istage)
end do
print([U=>c, V=>c], 1)
end timeloop
! end phase solve

ppm_finalize()
end client

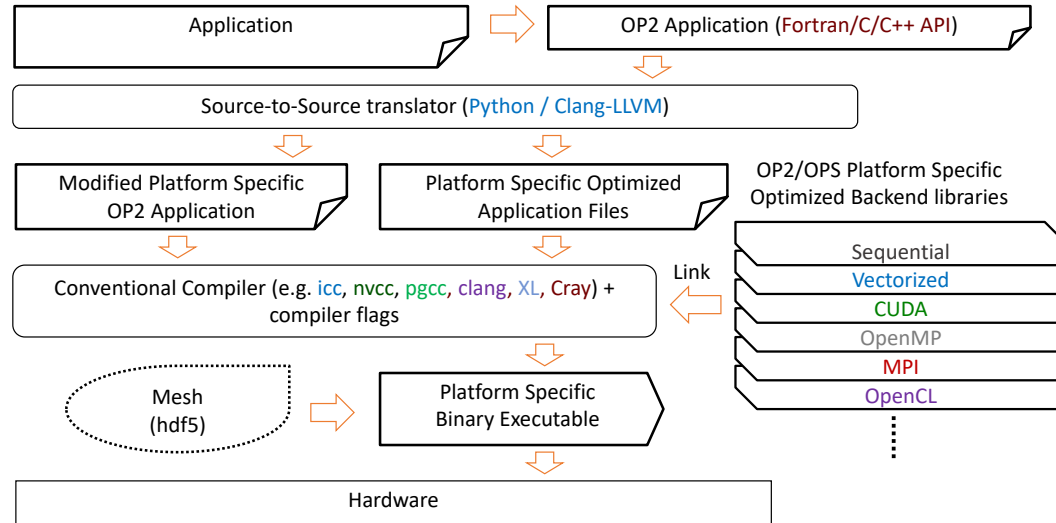
rhs grayscott_rhs_0(U=>c, V)
get_fields(dU_rhs_0, dV_rhs_0)

dU_rhs_0 = apply_op(L, U)
dV_rhs_0 = apply_op(L, V)
foreach p in particles(c) with sca_fields(U, V, dU_rhs_0, dV_rhs_0)
  dU_rhs_0_p = Du * dU_rhs_0_p - U_p * (V_p**2_mk) + F * (1.0_mk - U_p)
  dV_rhs_0_p = Dv * dV_rhs_0_p + U_p * (V_p**2_mk) - (F + kRate) * V_p
end foreach
end rhs
```



# Demonstrator Applications

## Mini-applications as DSL Demonstrators

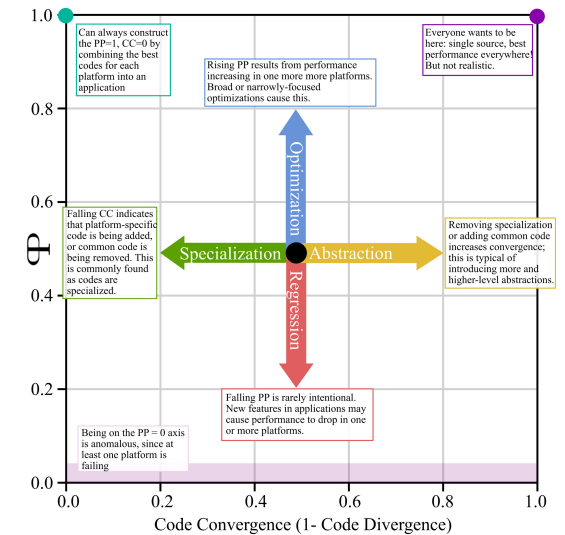
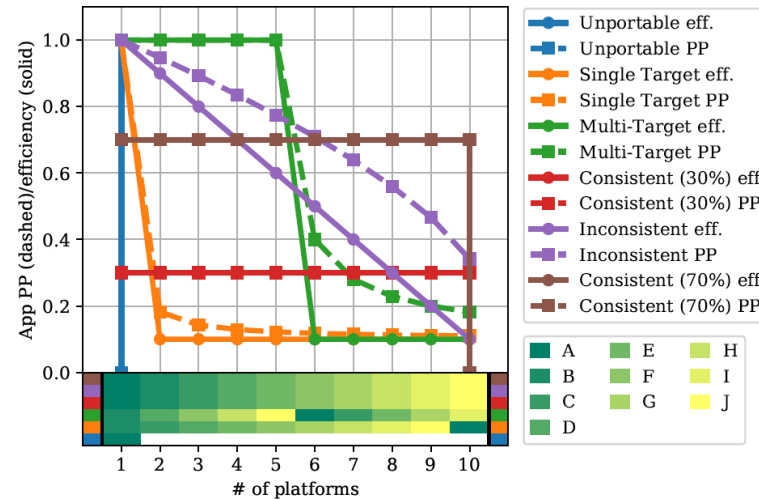
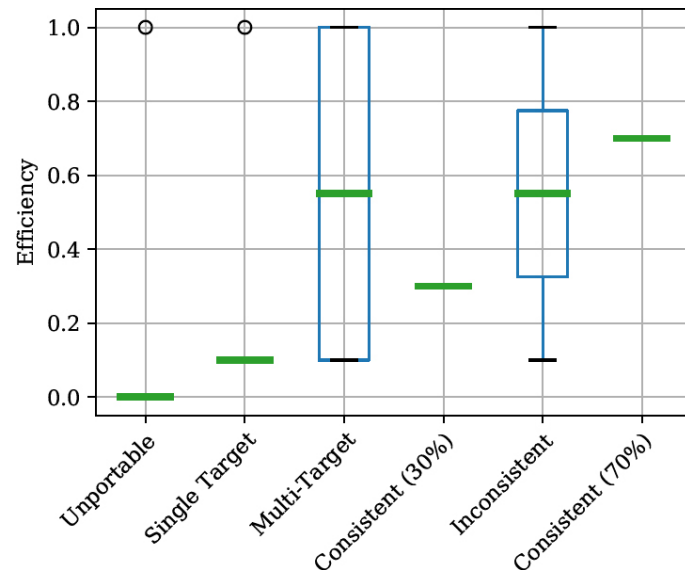


- We will develop miniaturised demonstrator applications in a DSL
- e.g. port mini-FEM-PIC
  - ... to a UKAEA-developed DSL
  - ... to OP2 w/ an implementation of our proposed particle DSL

# Demonstrator Applications

## Mini-applications as DSL Demonstrators

- Developed demonstrator application will be evaluated for performance and portability
- Evaluation will follow our current methodology
- Will additionally assess productivity of DSL [1]



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# Edge Physics Consultancy

Verification and benchmark calculations with existing plasma software

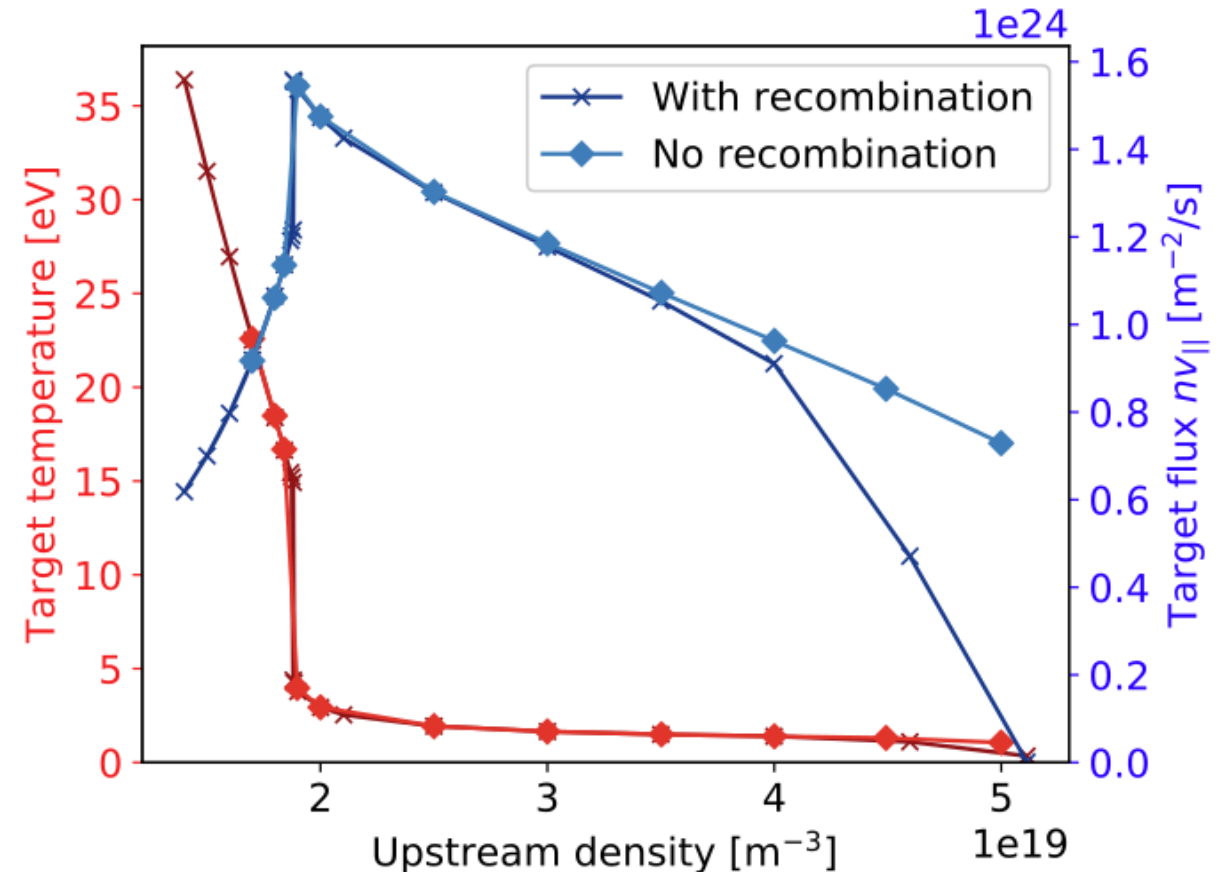
- Software tools – SD1D (& Hermes), EPOCH
- SD1D – 1D Fluid code readily extendible to include further physics modules (Hermes is same but 2D)
- EPOCH – Particle-in-cell code. Ab-initio kinetic physics for electrons and ions but lacks additional physics modules



# Edge Physics Consultancy

Verification and benchmark calculations with existing plasma software

- Activity 3.1/3.2 – identify edge physics test cases for 1D/2D system
- SD1D/Hermes have suite of example cases of varying complexity (steady state and transients)
- Example – benchmark temperature/flux on target for range of included physics packages
- Support with fully kinetic, particle-based EPOCH simulations

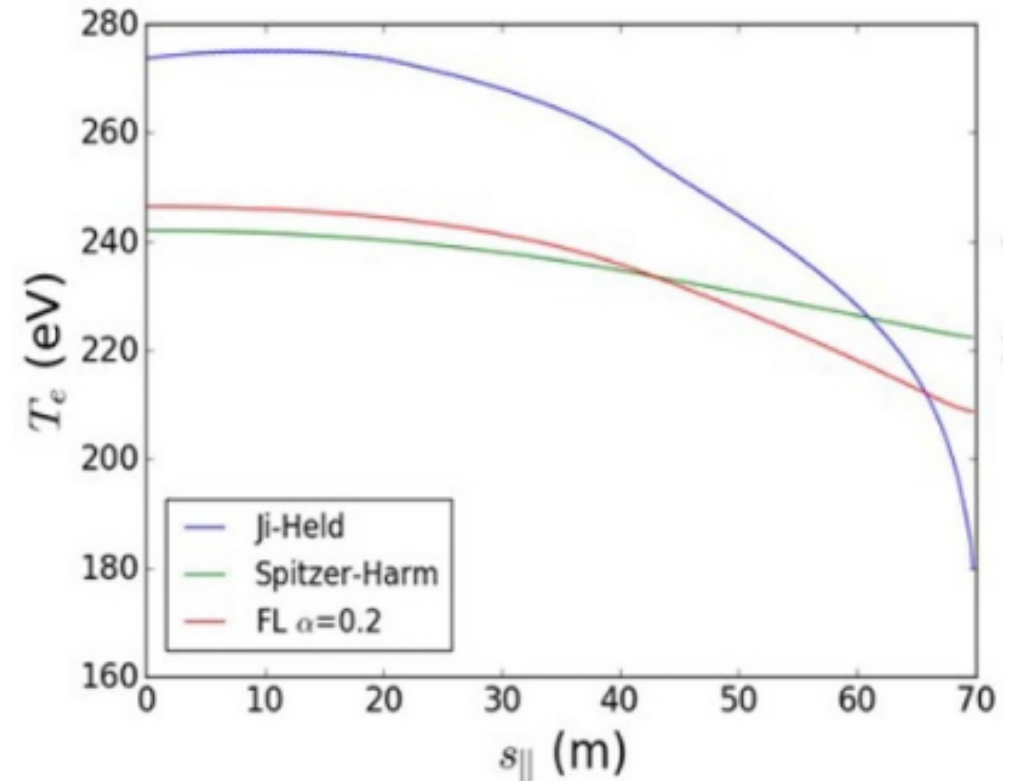


B. Dudson et al., PPCF, 61, 065008 (2019)

# Edge Physics Consultancy

Verification and benchmark calculations with existing plasma software

- Activity 3.3 - Explore mini-apps for incorporating kinetic effects in system 2-2
- Kinetic electron/neutral physics under development for SD1D/Hermes
- Validate against PIC and/or Vlasov Fokker Planck
- Models of different dimensionality. First step existing 1D kinetic electron transport models coupled to Hermes.



M. Wigram et al., Nucl. Fus., 60, 076008 (2020)

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