Coupling Codes at Exascale for the ExCALIBUR UKAEA NEPTUNE Nuclear Fusion Project

Ben Dudson, University of York

Thanks to Wayne Arter and Rob Akers, UKAEA

Towards Exascale Simulation of Integrated Engineering Systems at Extreme Scales

21 – 22 January, 2021

Outline

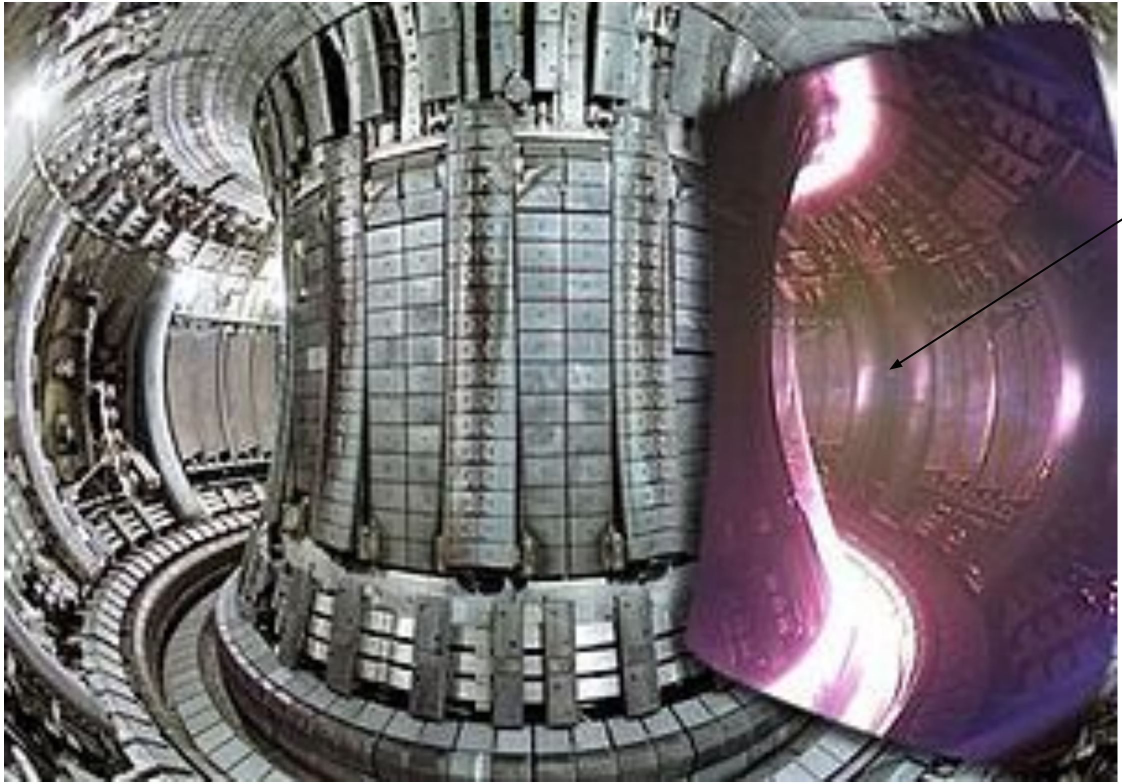
- **Neptune** will be a new code for modelling fusion plasmas
  - A unique opportunity to design a system from scratch

- A co-design effort
  - Advanced physics models valid in fusion reactor conditions
  - Exascale hardware, near-term and > 5-10 years
  - Scalable algorithms
  - Uncertainty Quantification for actionable outputs
  - Integration into engineering design and scientific data workflows

The aim here is to

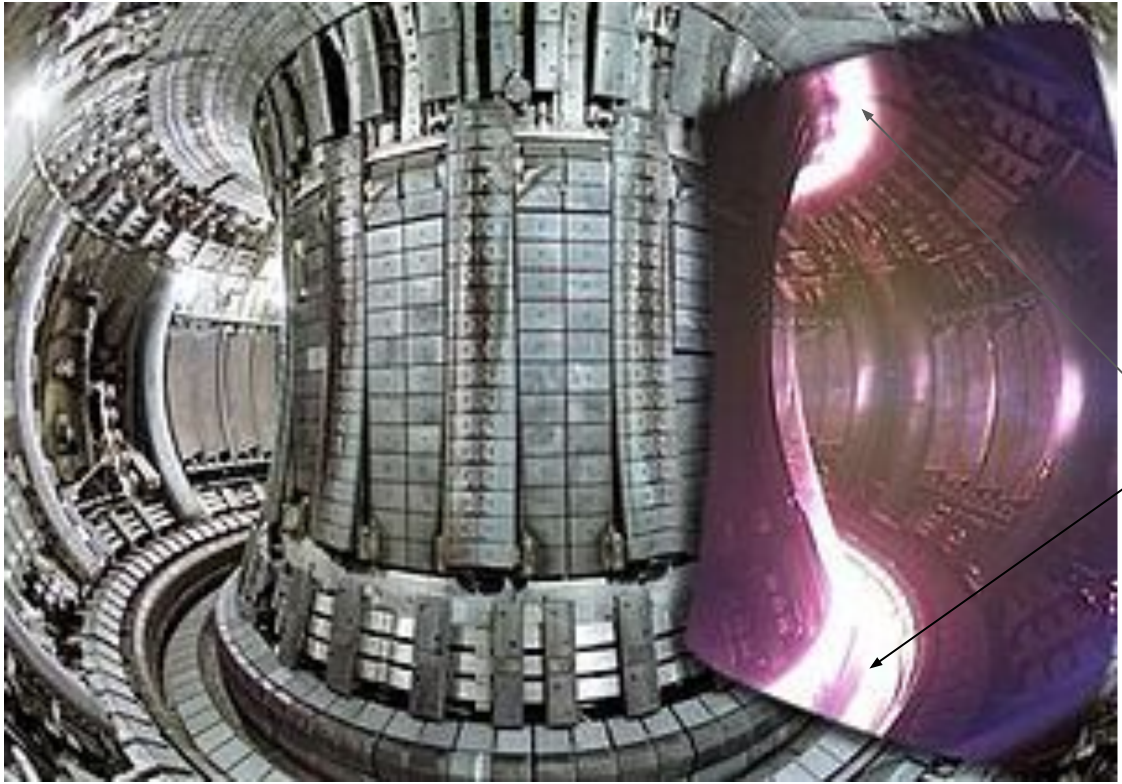
- Present the context, constraints, and previous work in this area
- Present developing ideas on coupling in Neptune
- Ask for feedback, suggestions, ideas for improvement
- Encourage you to get involved in the Neptune project!

Tokamaks are tightly coupled systems



Core plasma
Almost collisionless
Small fluctuations (1%)
Fast particles (3.5 MeV He)

Tokamaks are tightly coupled systems



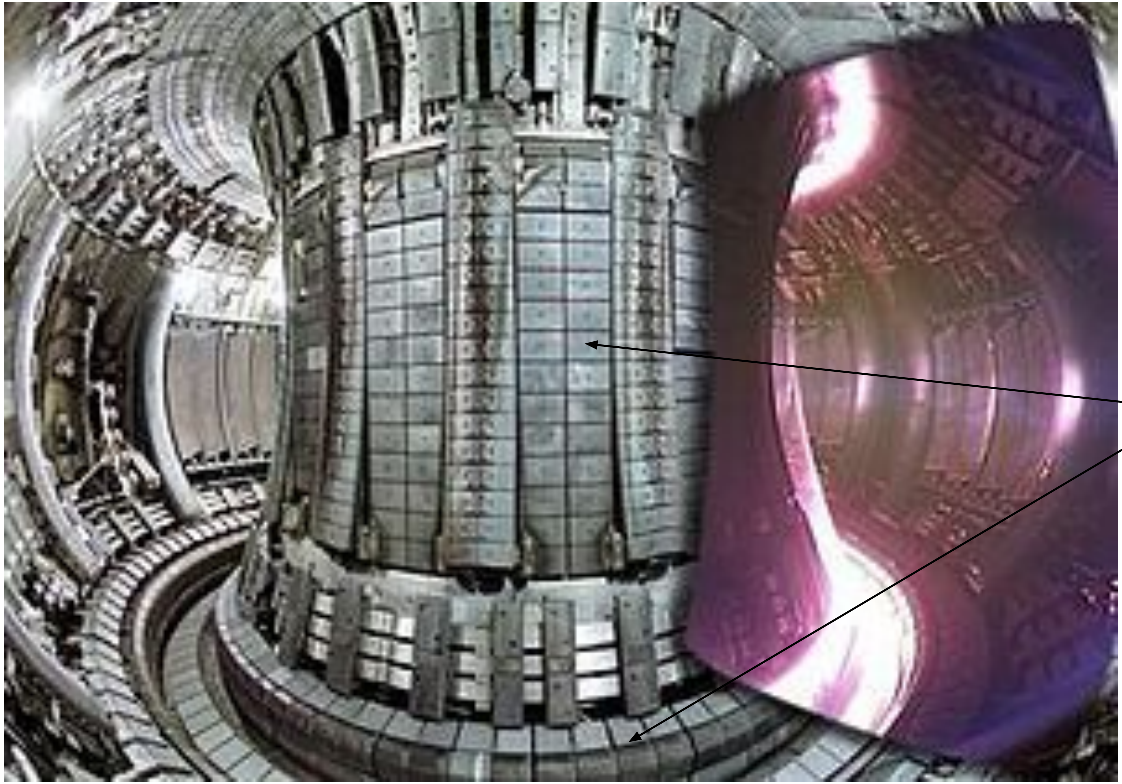
Divertor plasma
Collisional (partly)
Large fluctuations (>100%)

Neutral gas
Collisional -> collisionless

Impurity species
Be, C*, N*, Ne, Ar, W
* Not in a reactor

Vital for power handling:
Divertor “detachment”

Tokamaks are tightly coupled systems



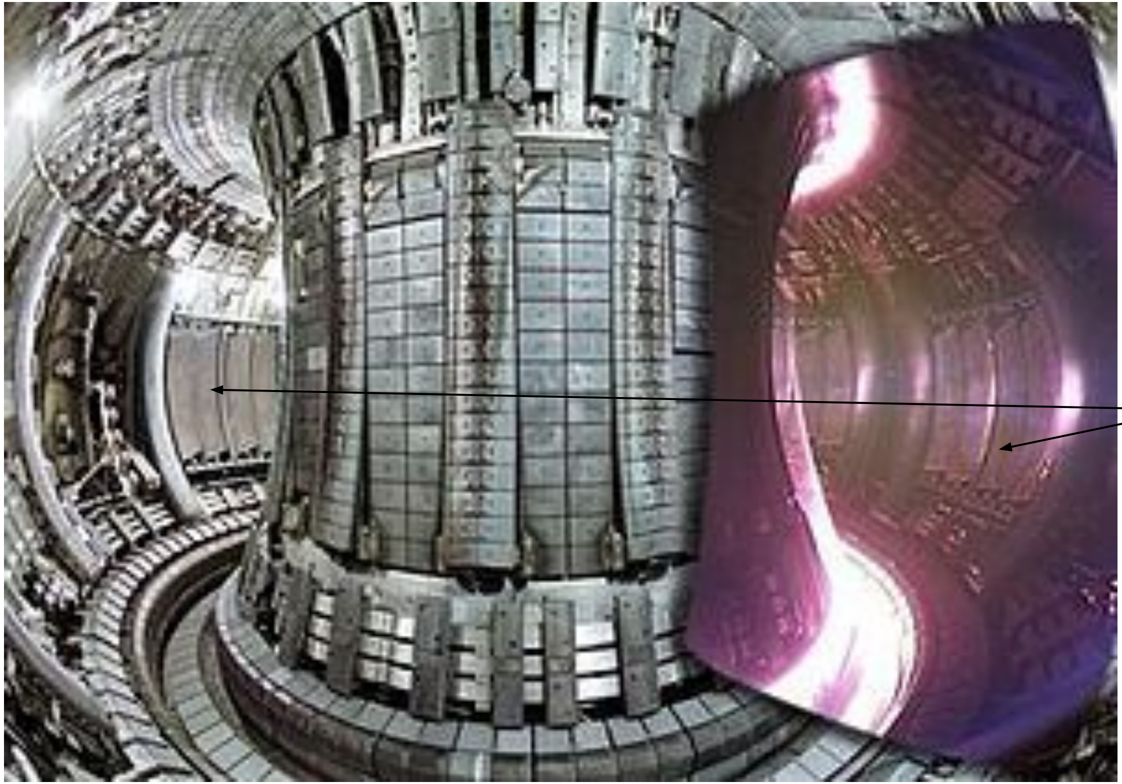
Surface materials

Heat, particle fluxes

Erosion, sputtering

Reflection, absorption
Changes plasma solution

Tokamaks are tightly coupled systems

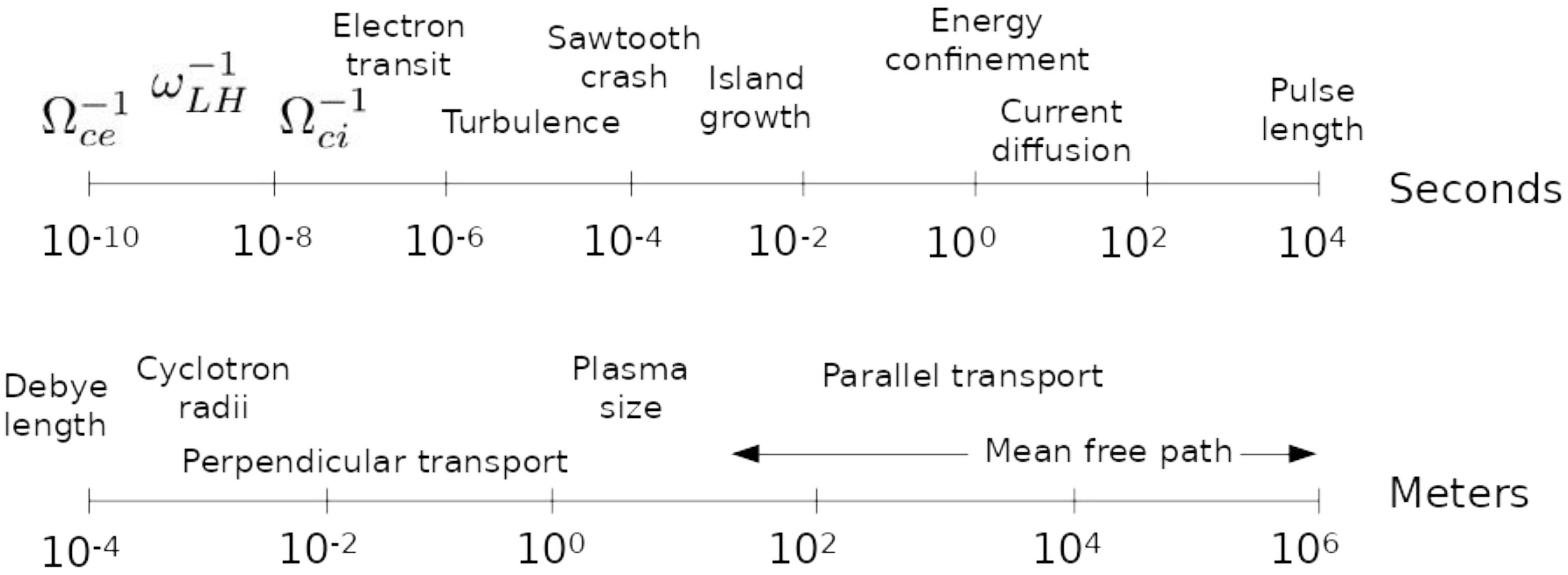


Plasma heating systems

EM waves
Fast neutral atoms

Absorption in plasma depends on plasma configuration

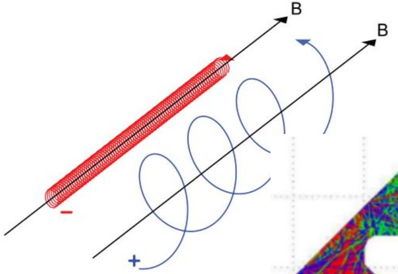
Large range of scales



Types of models

No model can solve this range of scales. Instead we have:

Fully kinetic models,
following individual particles on short time and length scales



Barnes-Hut trees
e.g. PEPC (Julich)

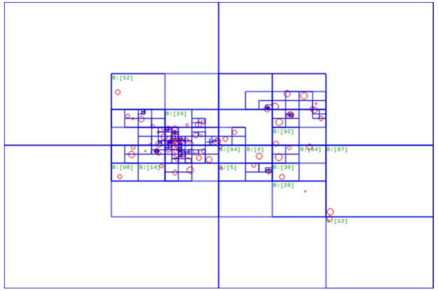
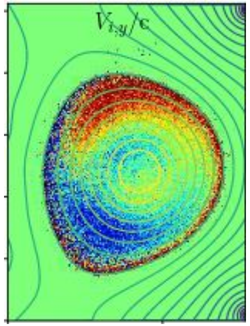
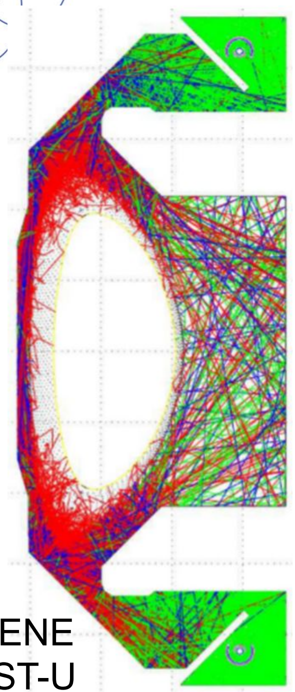


Image: Wikipedia

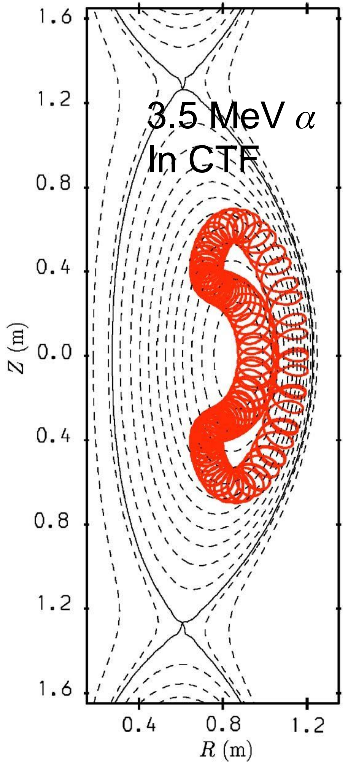
6D structure-preserving
geometric PIC



J Xiao, H Qin
arXiv:2004.08150



EIRENE
MAST-U



K. G. McClements Physics of Plasmas 12, 072510 (2005);
https://doi.org/10.1063/1.1936532

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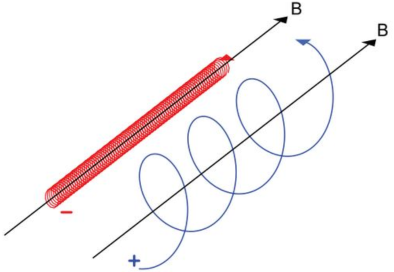
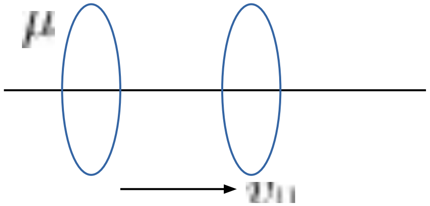
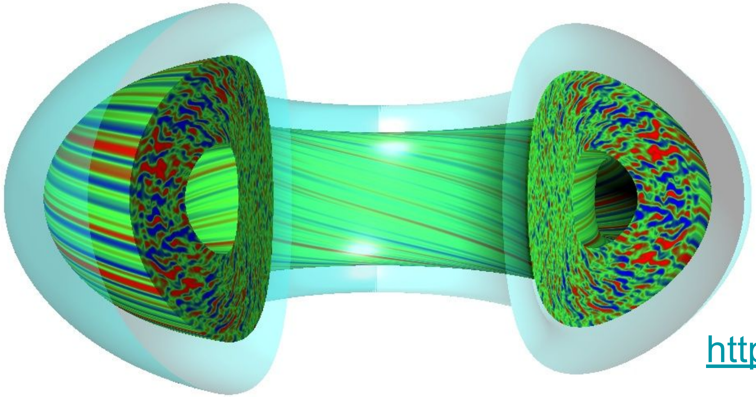


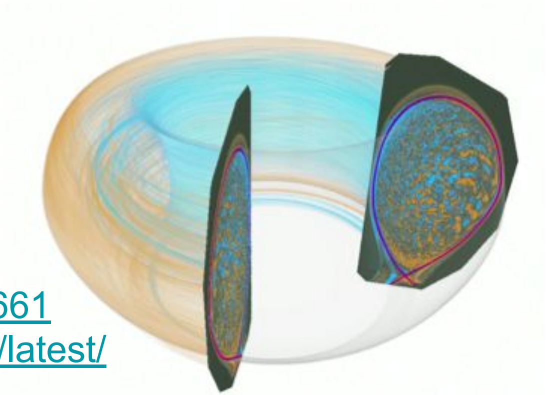


Gyro-kinetic models which average over the shortest time scales



Continuum <-> PIC

Coupling: WDMapp
G. Merlo et al. 2021
https://doi.org/10.1063/5.0026661
https://wdmapp.readthedocs.io/en/latest/



GYRO, https://w3.pppl.gov/~hammett/viz/viz.html

XGC, https://hbps.pppl.gov/

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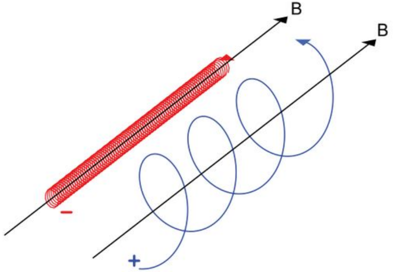
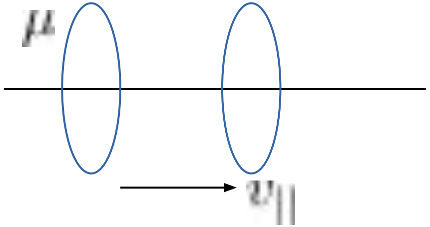
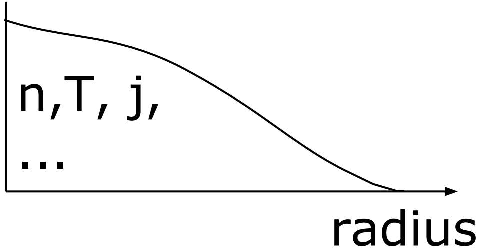
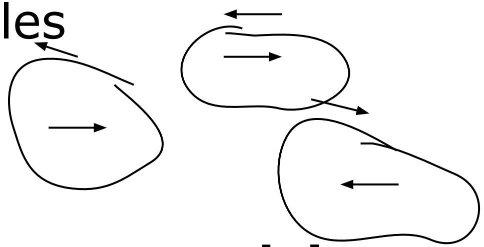




Gyro-kinetic models which average over the shortest time scales

Fluid models, averaging over small length and time scales



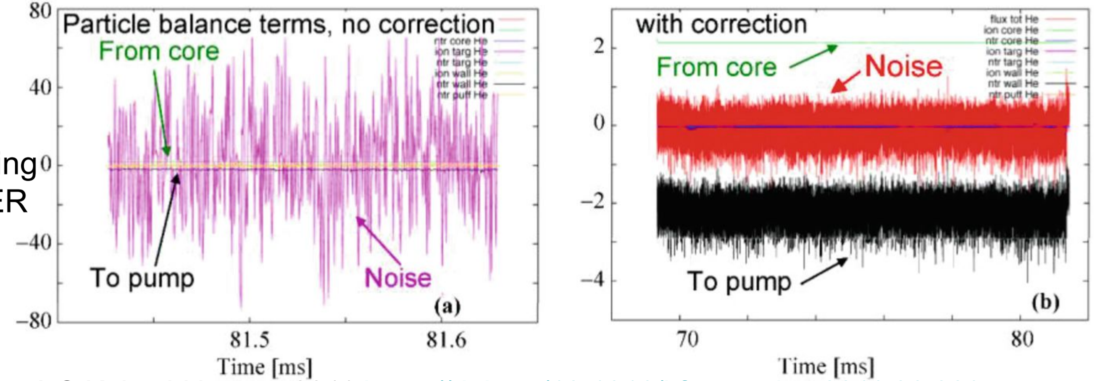


Transport models, averaging over turbulence timescales

SOLPS = B2 (fluid) + EIRENE (MC)

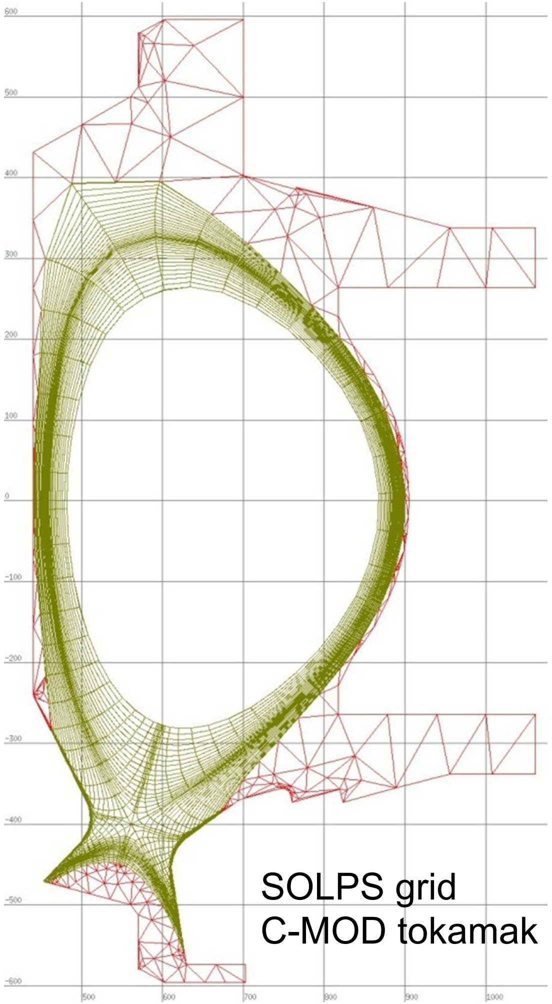
- Widely used for experimental interpretation, planning, and machine design (eg. ITER, STEP)
- Evolved to steady state
    - Loose coupling of fluid and neutral models
    - Still takes ~ months for ITER runs
- Requires careful handling of Montecarlo noise

He Pumping in ITER



A S Kukushkin et al 2011 https://doi.org/10.1016/j.fusengdes.2011.06.009

V.Kotov 2017 https://doi.org/10.1063/1.4980858

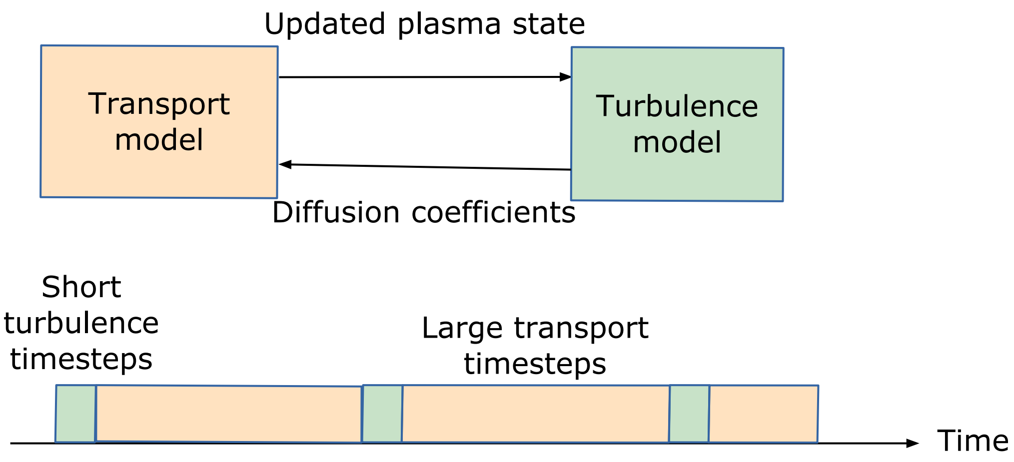


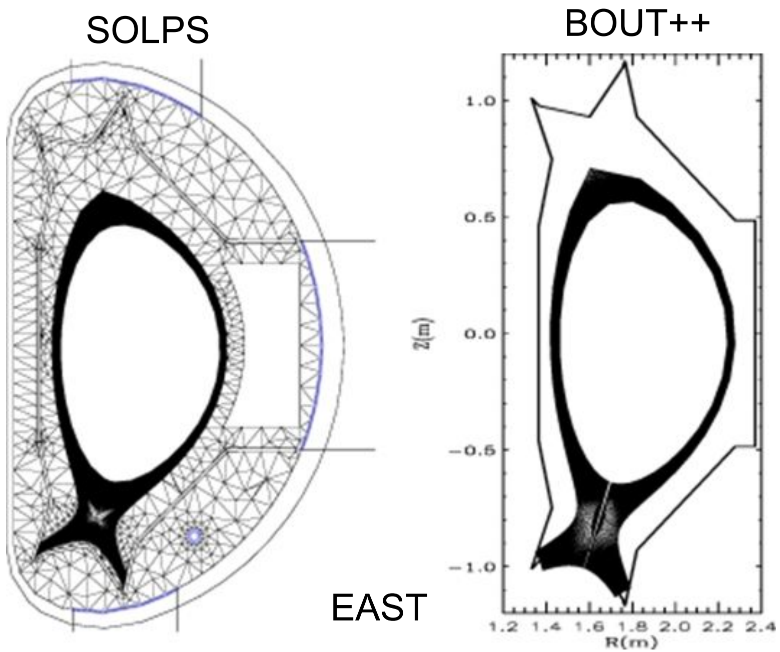
SOLPS grid
C-MOD tokamak

https://www.iter.org/newsline/-/2168

Coupling turbulence simulations

1. Transport and turbulence simulations in the same spatial domain



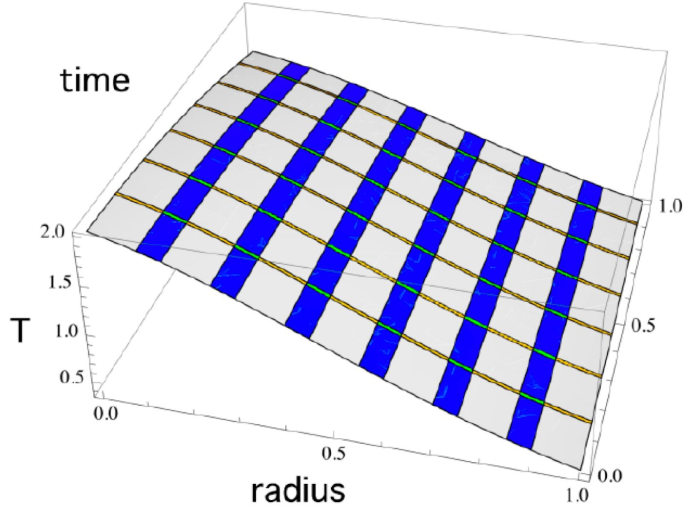


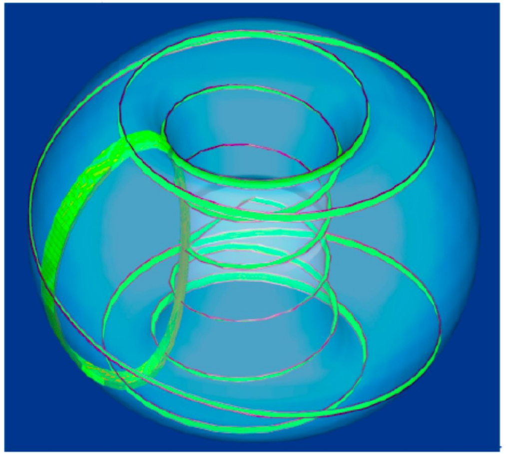
Type of surrogate model coupling (diffusion processes < turbulence)

D. R. Zhang et al Physics of Plasmas 26, 012508 (2019); https://doi.org/10.1063/1.5084093
D.R. Zhang *et al Nucl. Fusion* **60** 106015 (2020) https://doi.org/10.1088/1741-4326/abaa90

Coupling turbulence simulations

1. Transport and turbulence simulations in the same spatial domain
2. Transport and turbulence in non-overlapping domains





TRINITY (M.Barnes et al) http://www-thphys.physics.ox.ac.uk/people/mbarnes/projects/trinity/

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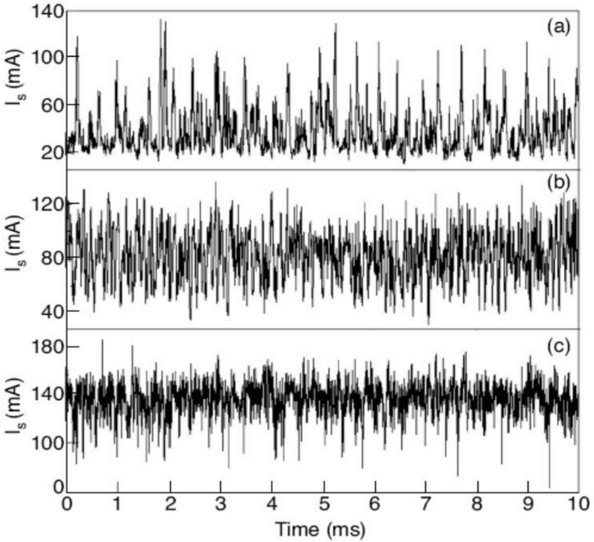
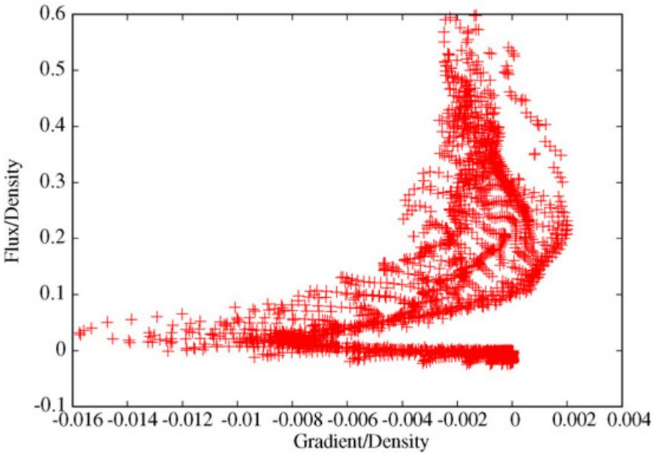
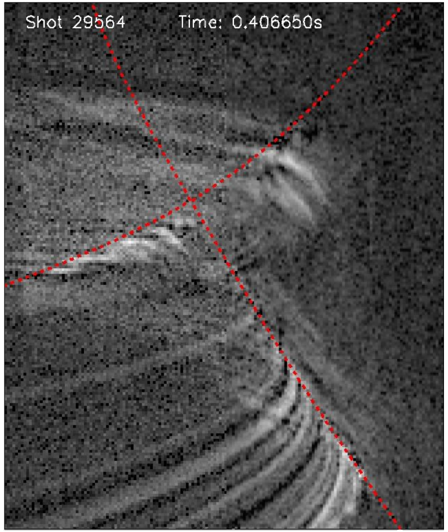


JET data. D'Ippolito et al 2011



V.Naulin 2007



MAST, J.Harrison

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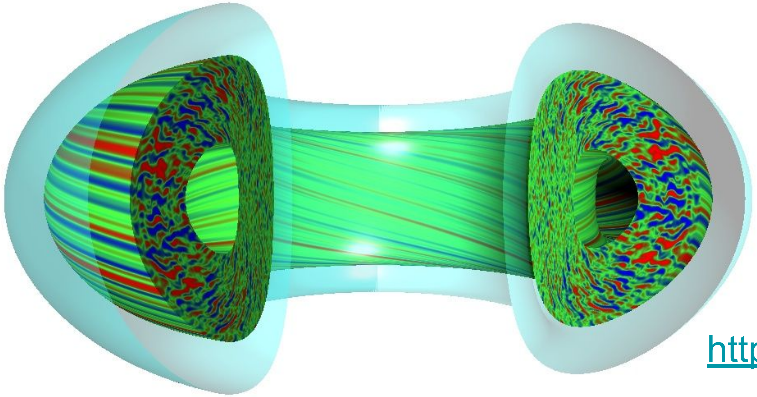
Coupling turbulence simulations

1. Transport and turbulence simulations in the same spatial domain
2. Transport and turbulence in non-overlapping domains
3. Turbulence simulations on neighbouring domains

- Electromagnetic field solve spans domain -> Coupling not only through boundary fluxes
- Overlapping domains (handshake), blending of charge densities
- Mapping between meshes

Errors, conservation properties?



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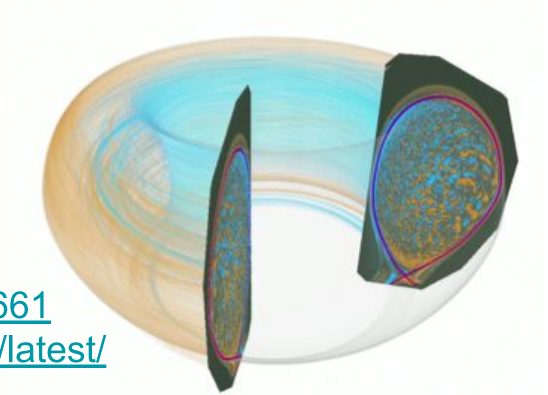
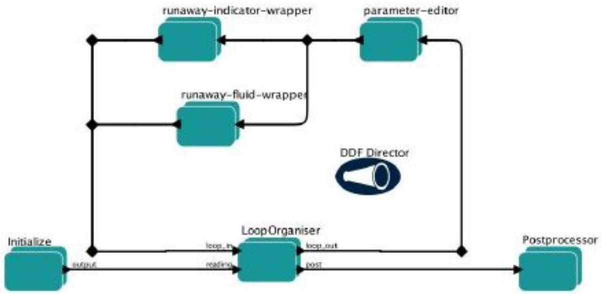


XGC, https://hbps.pppl.gov/

Integrated modelling

- Loose coupling between multiple components
  - Often iterative eg interaction of sources and time-varying mean profiles
  - Each component is run in turn (conceptually), keeping others fixed (Picard iteration)
- Usually work at a high level, reduced dimensionality
- Several past and present well-funded efforts (e.g. Proto-FSPs)

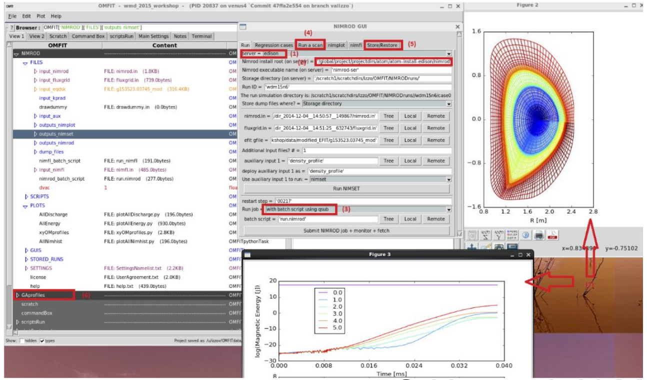
ITM - Kepler framework



Gergo I. Pokol et al 2019 Nucl. Fusion 59 076024

https://wpcd-workflows.github.io/

OMFIT - ATOM



C.Holland, NIMROD

https://gafusion.github.io/OMFIT-source/

Challenges

1. Different physical models
2. Different grids
3. Implicit time-step coupling
4. Long-range electromagnetic effects
5. Important small differences between large quantities

<u>Exascale</u>

6. Minimising global comms
7. Redundancy / failover
8. Data management

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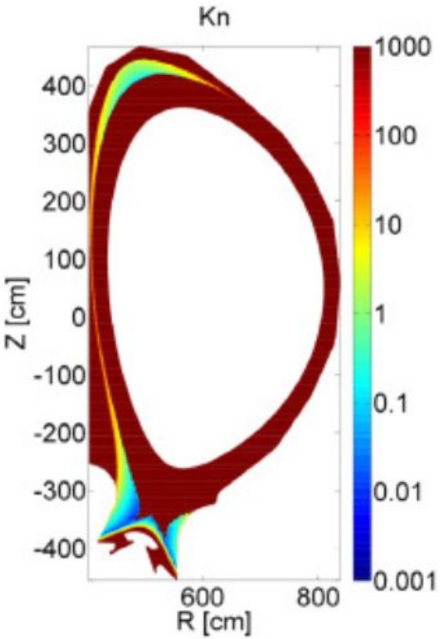
- Kinetic (5 or 6D) to fluid (2 or 3D)
- Fluid - kinetic hybrid neutrals



Wide range of Knudsen number (ITER, SOLEDGE2D)

M.Valentinuzzi et al 2018, https://doi.org/10.1016/j.nme.2018.12.003

AP schemes

See also:

N Horsten, PhD 2019 https://lirias.kuleuven.be/retrieve/533094

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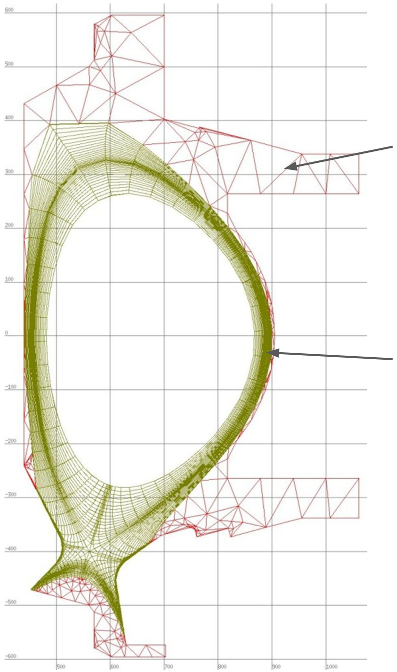
- Plasma is affected by magnetic field; neutrals are not



SOLPS grid
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https://www.iter.org/newsline/-/2168

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- Wide range of overlapping scales
    - Fast waves e.g fast magnetosonic
    - Electrons vs impurity ion masses
    - Neutral gas reaction rates very sensitive to plasma state, strongly impact plasma
- Different time-stepping methods
    - Plasma fluids: implicit or semi-implicit
    - Particle methods usually explicit
- May require implicit coupling
  I.Joseph et al 2017 https://doi.org/10.1016/j.nme.2017.02.021
- Coupling to surrogate models may enable asynchronous operation
  (c.f. Fluid neutrals, kinetic corrections)

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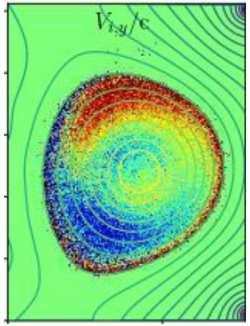
- Plasma models evolving E, B fields contain short time-scales
- Plasmas are essentially incompressible in 2D (perp. To B)
- Requires an elliptic solve at every timestep (global coupling), or sub-lightspeed timesteps (~ps)



J Xiao, H Qin
arXiv:2004.08150

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- Large forces (MN), small mass (g)
- Neutral-plasma exchange with sensitive atomic rates (c.f. combustion)
- Quasineutrality: Electric field determined by small difference in large currents

$$\partial_t \omega^\epsilon + \frac{1}{\epsilon}\{\omega^\epsilon, \Psi^\epsilon\} = (\Delta\omega^\epsilon - \Delta\omega_{eq})$$

$$-\Delta\Psi^\epsilon = \omega^\epsilon \,.$$

"singularly-perturbed problem"

- Asymptotic-Preserving schemes

B Fedele 2019 https://hal.archives-ouvertes.fr/hal-02303653

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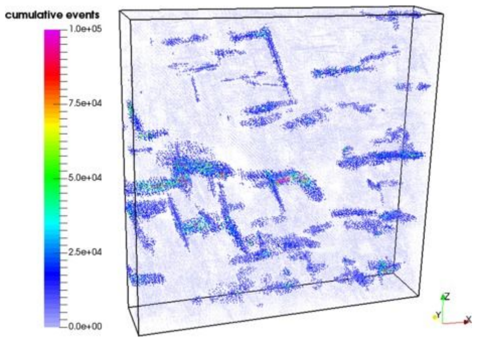
- Asynchronous time-stepping

  Space-time meshes, ADER DG

  J.E. Flaherty et al 1997 https://doi.org/10.1006/jpdc.1997.1412
  A Taube et al 2008 https://doi.org/10.1002/jnm.700
- Asynchronous multi-level methods
- Sub-stepping
- Surrogate models, with on-the-fly training
- Discrete Event Simulation

  Requires roll-backs to maintain causality

  Q Shao et al 2019 https://doi.org/10.1016/j.jcp.2019.01.026



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- Recovery of partial solves
  - Reconstruction
  - Duplication
- Checkpointing / restarting

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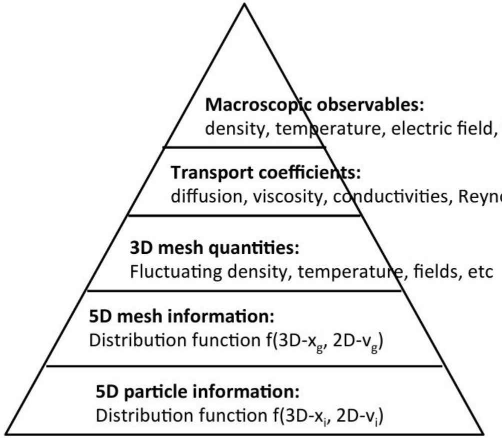
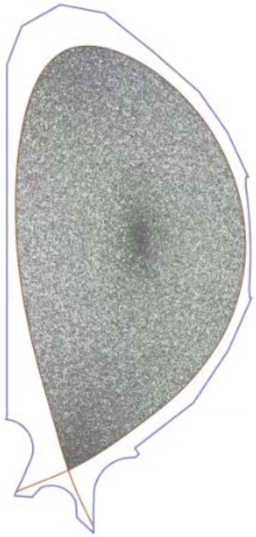
- Large volume of data
  - PIC codes particle data

    E.g. XGC
    640B particles on 64M grid cells
    Single check-point ~100TB
    Turbulence run >100PB per day
  - Continuum codes 5D grid
- In-memory analysis
  - Data reduction, compression





C.S.Chang 2017, https://theory.pppl.gov/news/invited/20171117Chang.pdf

Conclusions

- The fusion plasma system is hard to disentangle
  - There are strong couplings (bi/multi-directional) between sub-components which lead to time-step limitations or numerical instabilities
  - There are rarely clear scale separations, but a continuum
  - Historically the most successful approaches have tended to be tightly integrated (e.g. XGC in the US FSP programme)

- Surrogate models offer the possibility to decouple components
  - Physics-based surrogates have been tried successfully
  - A scalable system needs to minimise global synchronisation, communications
  - Asynchronous online training of models based on evolving conditions
  - Likely also essential for sensitivity analysis and UQ.

- An interesting and important problem
  - Suggestions, and involvement in the project welcome!