Software Engineering for Fusion Reactor Design

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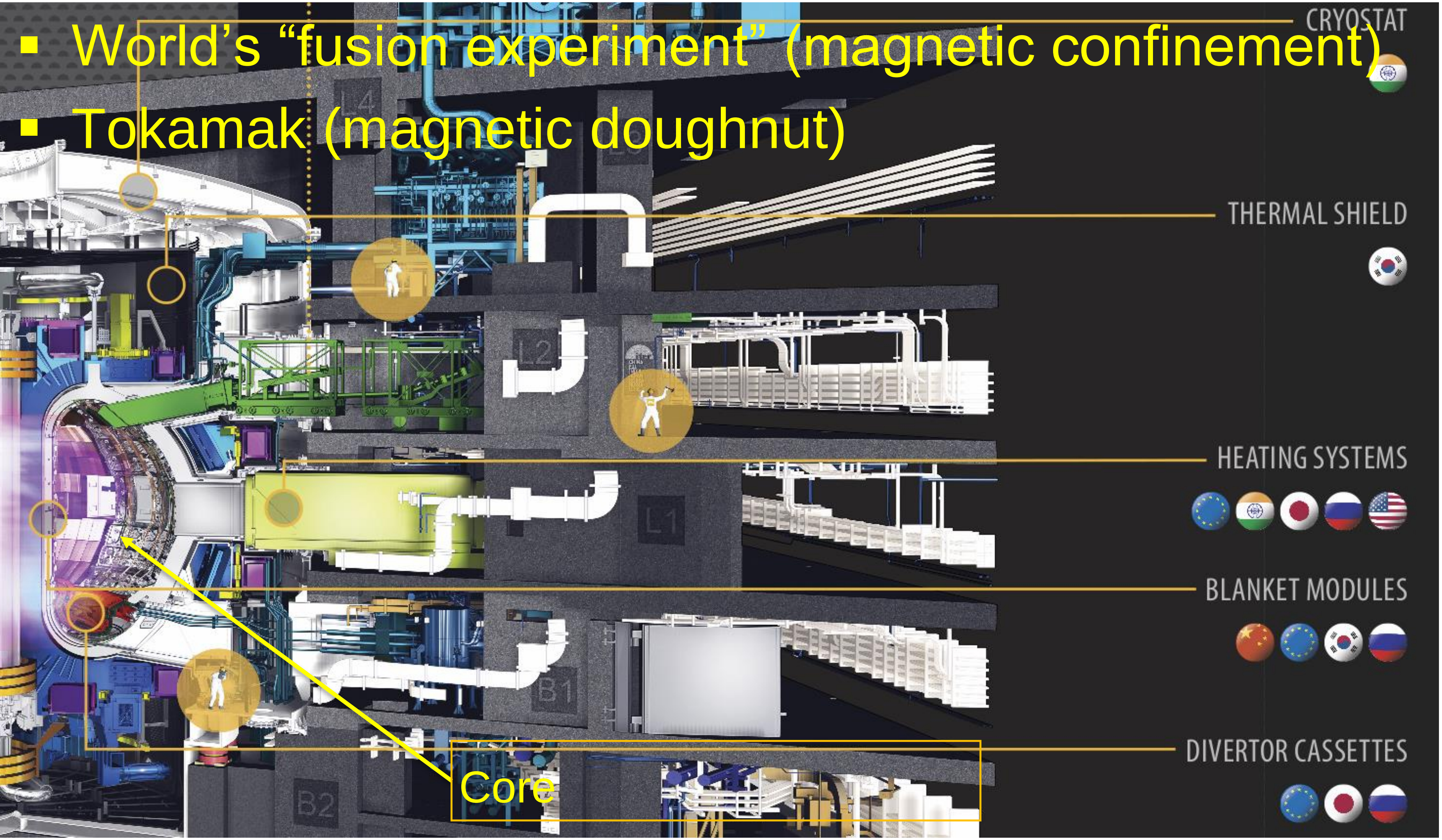
Outline

Show how we have produced software capable of further development after 30+yr:

1. Background, the ITER experiment.
2. History of scientific software tools at Culham.
3. Designing one piece of software for 30+ years of development and use by ITER.
4. Producing a more comprehensive reactor design tool.

ITER

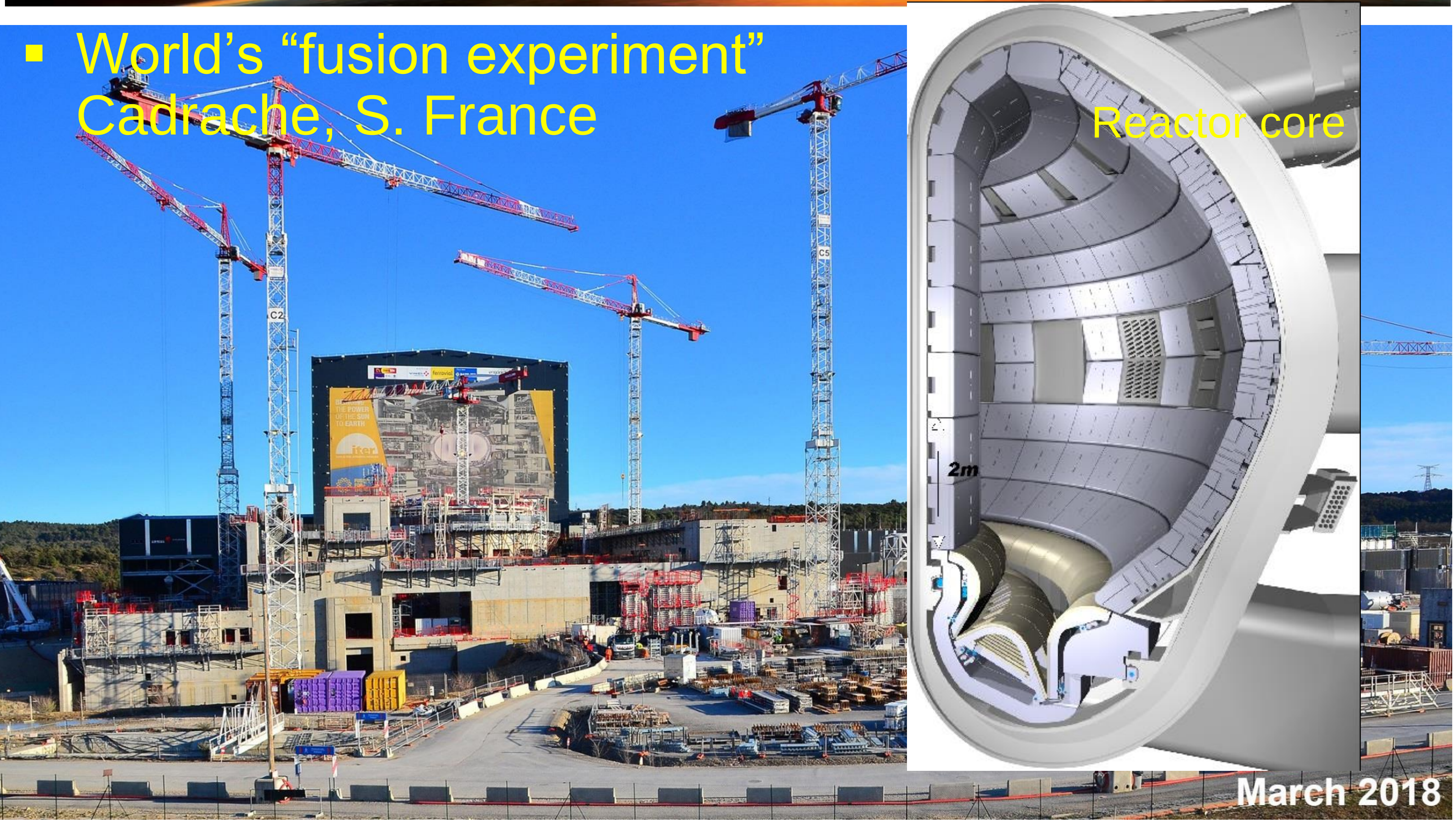
- World's "fusion experiment" (magnetic confinement)
- Tokamak (magnetic doughnut)



www.iter.org

ITER site today

- World's "fusion experiment" Cadrache, S. France



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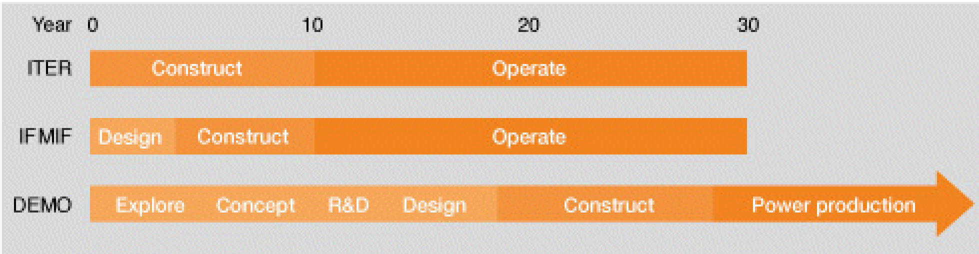
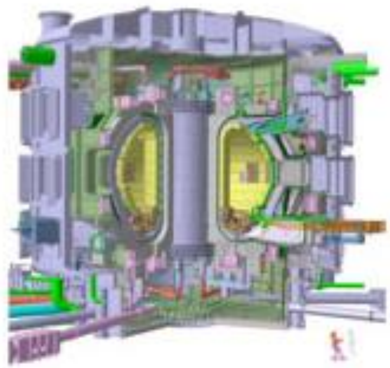
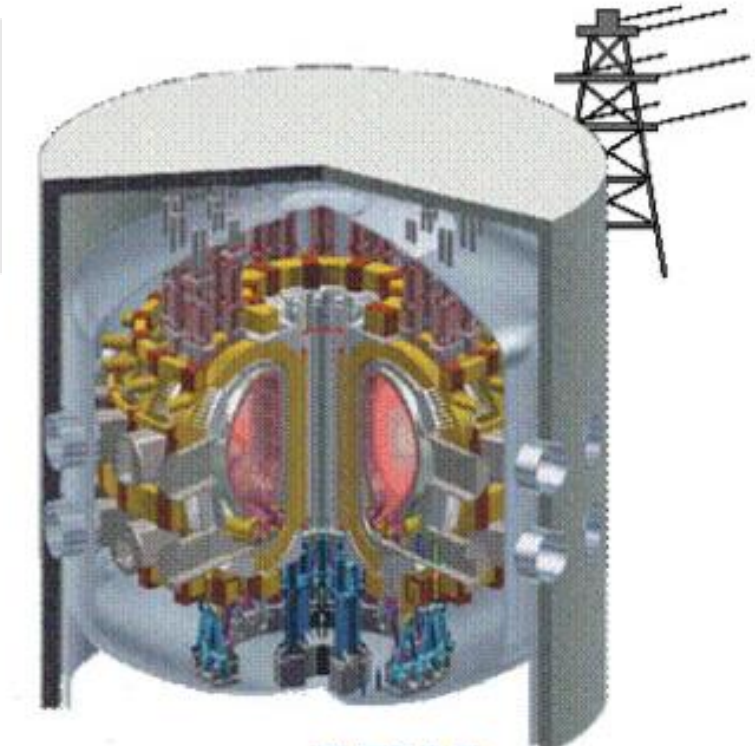
Towards Electricity Generation







JET

80 m³

~16 MW_{th}

ITER

800 m³

~ 500 MW_{th}

DEMO

~ 1000 - 3500 m³

~ 2000 - 4000 MW_{th}

iter.org ccfe.ac.uk

History of scientific software tools at Culham

Scientific Software at Culham

Leading players

- K.V.Roberts (to 1983)
  - 1969 established journal Computer Physics Communications (CPC, Impact factor 3.9)
  - CPC Program Library
  - “Software should be readable like a book” [2]
- J.W. Eastwood (to 1996)
  - Further developed OLYMPUS programming system, became U(nix)-OLYMPUS c.1990
  - “Computer Simulation Using Particles” with Roger W. Hockney, P^3M algorithm, 3DPIC/EMX

U-OLYMPUS

U-OLYMPUS codes from mid-1980s are still capable not only of use but also of *development*.

- Basically strict FORTRAN 66 standard with minimal extensions for character handling.
- *Same language also* for preprocessing software, for code generation and formatting.
- *Same language* for graphics (Culham GHOST).
- C-shell wrapper, including makefile, version control via SCCS.
- Descriptive publications, man pages in troff/nroff

Fortran 77, 95, 2003 et seq

- New Fortran standards address many of deficiencies met by U-OLYMPUS
- Insufficient resource/gain to update U-OLYMPUS
- Concentration on programming style after Brealey, now object-oriented, see ref. [1] of abstract, ie. Report CCFE-R(15)34, and templates at

https://github.com/wayne-arter/smardda-qprog.git

- C shell -> Bash shell utilities, including git for version control and general provenancing.

Section 3

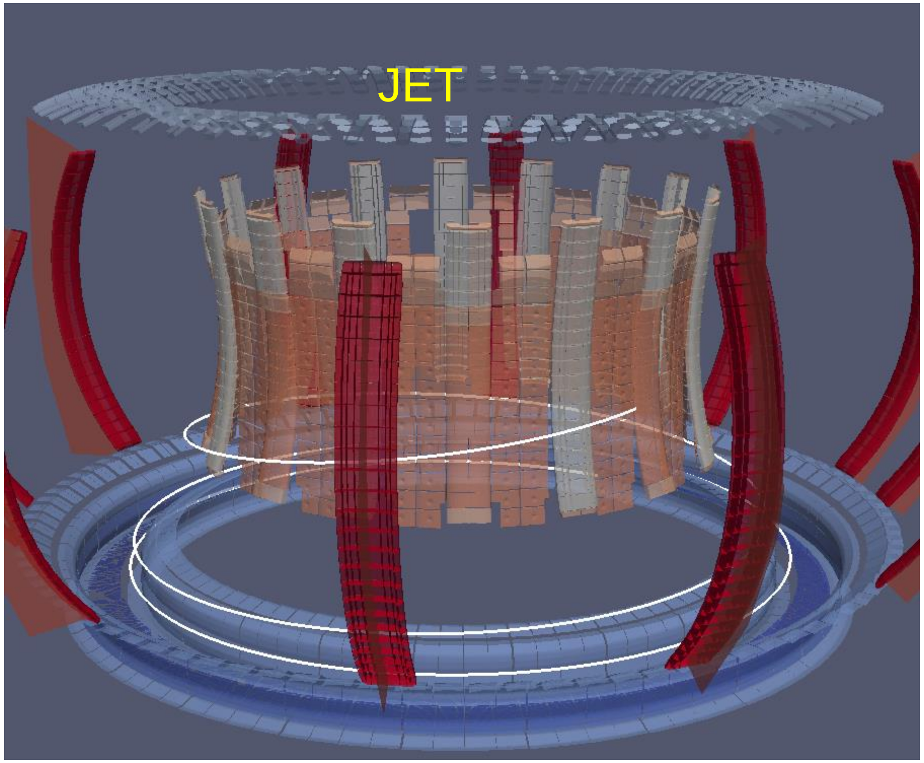
My contribution to ITER

ITER Projects 2012 and 2015/16

- Confinement of plasma in tokamaks is not perfect and MegaWatts (MW) of energy expected to leak from outer midplane region – both projects to model “where power goes”
- Simple physics that power flows along fieldlines to “first” wall/plasma facing components (PFCs).
- Magnetic field-line tracing over complex geometry
- Up to 10^6 field-lines each as up to 10^5 rays using hybrid SMART/DDA algorithm (SMARDDA)

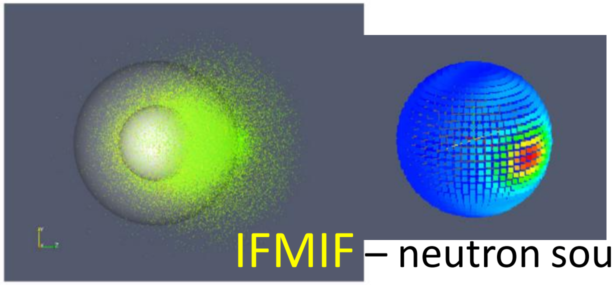
SMARDDA Software

- 21st Century development, started 2008.
- Modular object-oriented software based around the SMARDDA ray-tracing algorithm for triangulated surface geometries
- Written to own published Fortran-95 software standard [1]
- Documented in 2 publications
- Originally for neutronics and neutral beam duct design, adapted for ITER in SMITER project, now being used for reactor design, coupled to COSSAN sensitivity analysis/UQ software
- Linux/Mac ifort and gfortran + bash 3.0

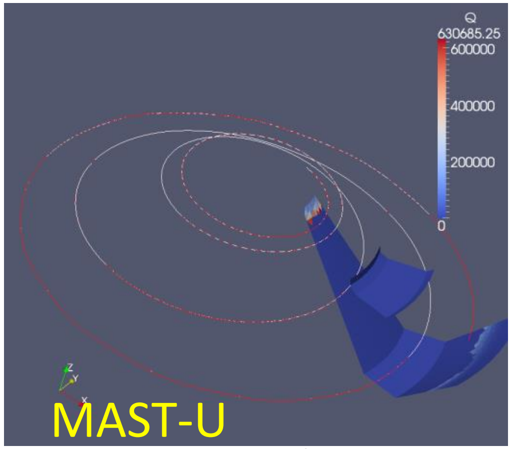


2 372 343 triangles

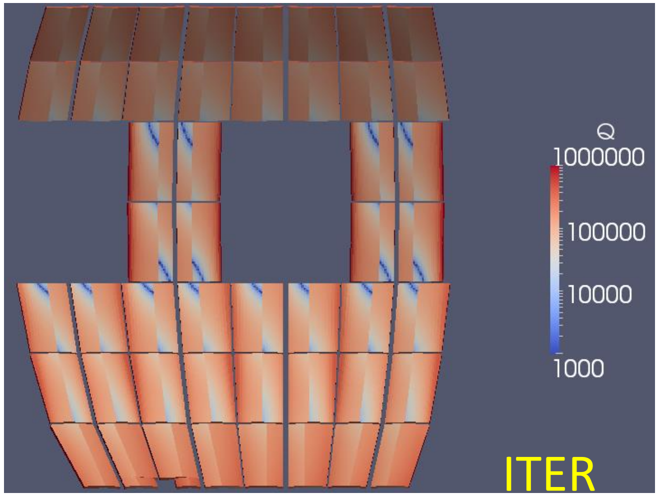
Applications of SMARDDA Modules



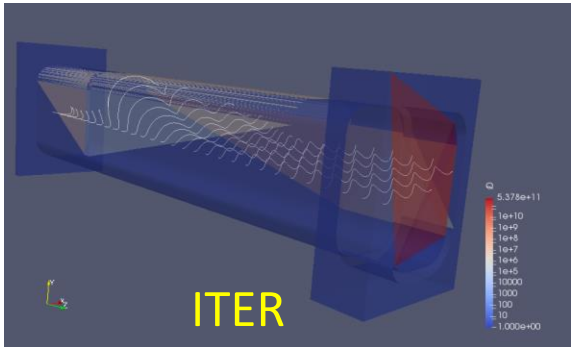
IFMIF – neutron source



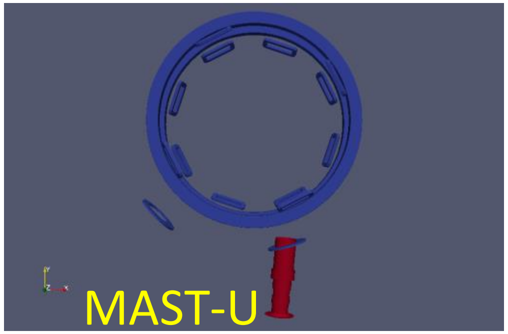
Divertors and Limiters

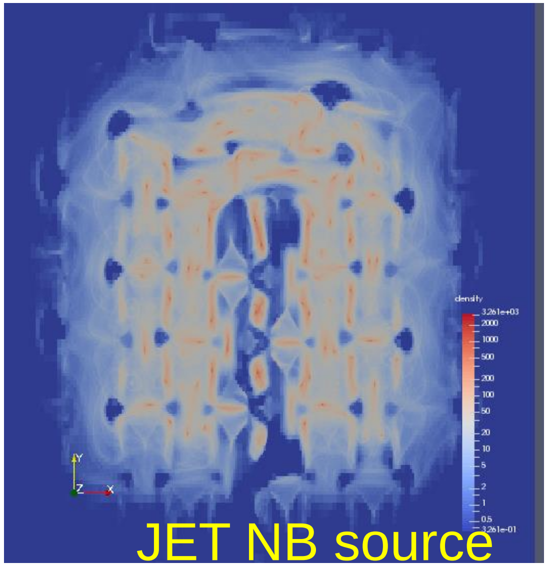


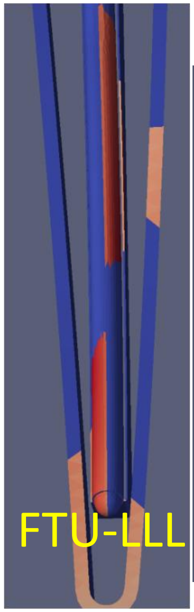
Power deposition on PFCs

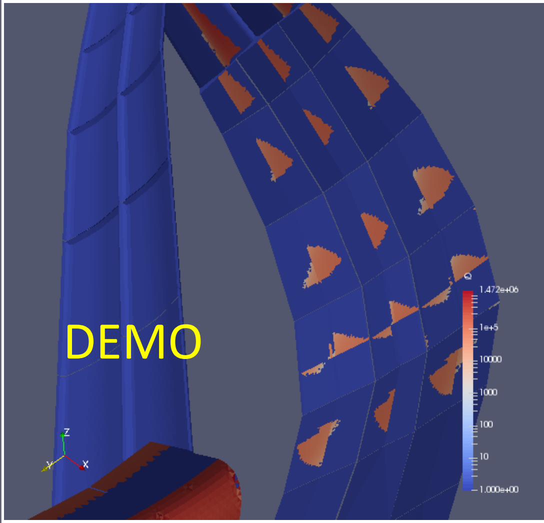


Neutral Beam Ducts - reionisation









SMITER (SMARDDA for ITER)

Specifications from customer

- User-friendly interface with GUI
- (Integration into ITER code-base IMAS)
- Capabilities for
  - Verify existing designs as physics basis improves
  - Interpret data from experiments (2025 on)
  - Integrate into real-time control system
- CCFE constraint that SMARDDA modules remain usable for commercial fusion reactor design, i.e. capable of integration into suite of engineering tools such as ANSYS.

SMITER (SMARDDA for ITER) 2

History implied:

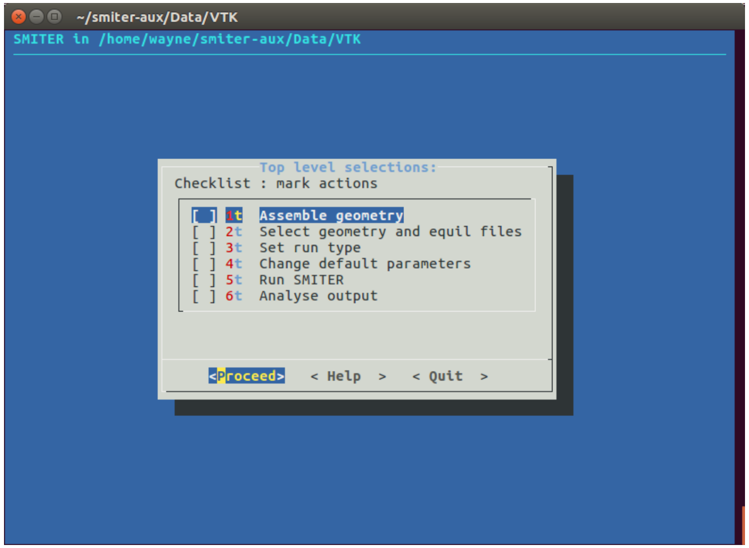
- Use of object-oriented Fortran 95 programming style
- Bash 3.0 wrapper including makefile
- Semi-personal awk/sed/grep development tools (not part of deliverable) for code generation

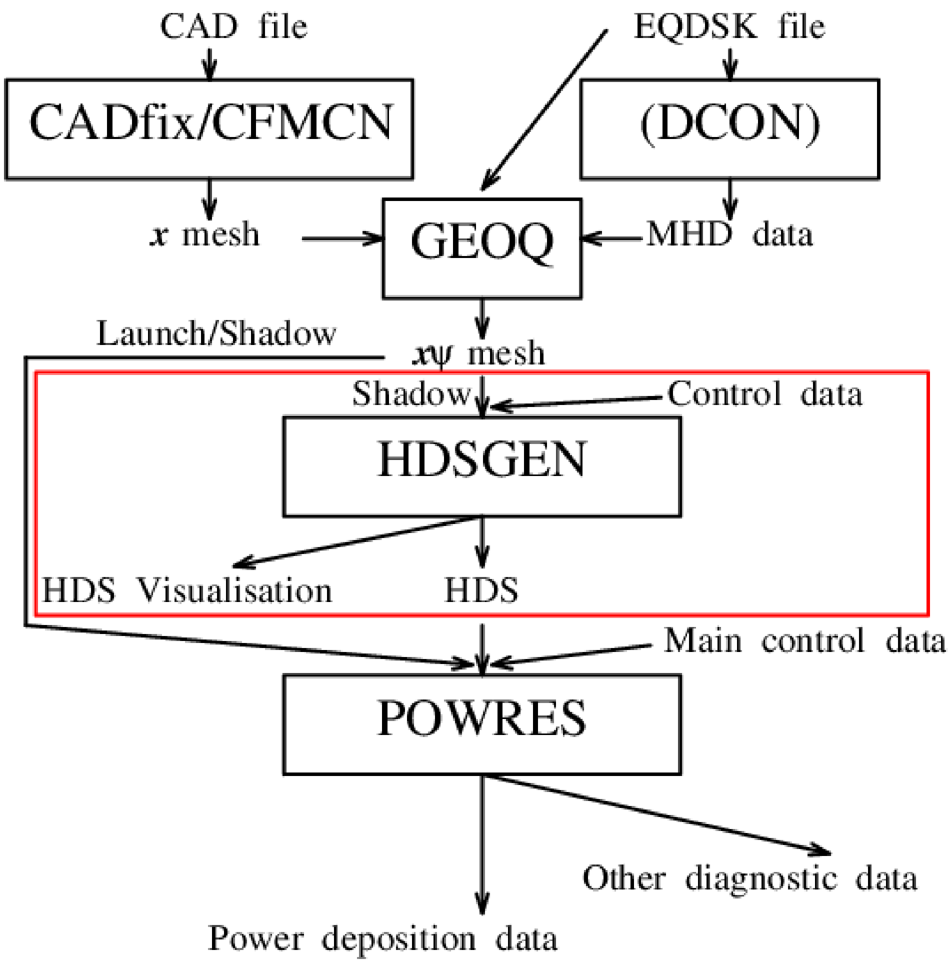
Additionally:

3-D surface meshes as legacy .vtk, from CATIA™ output of NASTRAN™ .dat geometry files. Implies visualisation by ParaView (and gnuplot).

SMITER kernel

- Set of Fortran-95 objects orchestrated by bash 3.0 script
- Unix dialog used for GUI, “training only”





Separate git repo for Fortran/bash source and for data for each project

- Project Script
- COSSAN UQ tool

Run Script (single case)

Cmdwrap (logging)

Fortran-95 executable

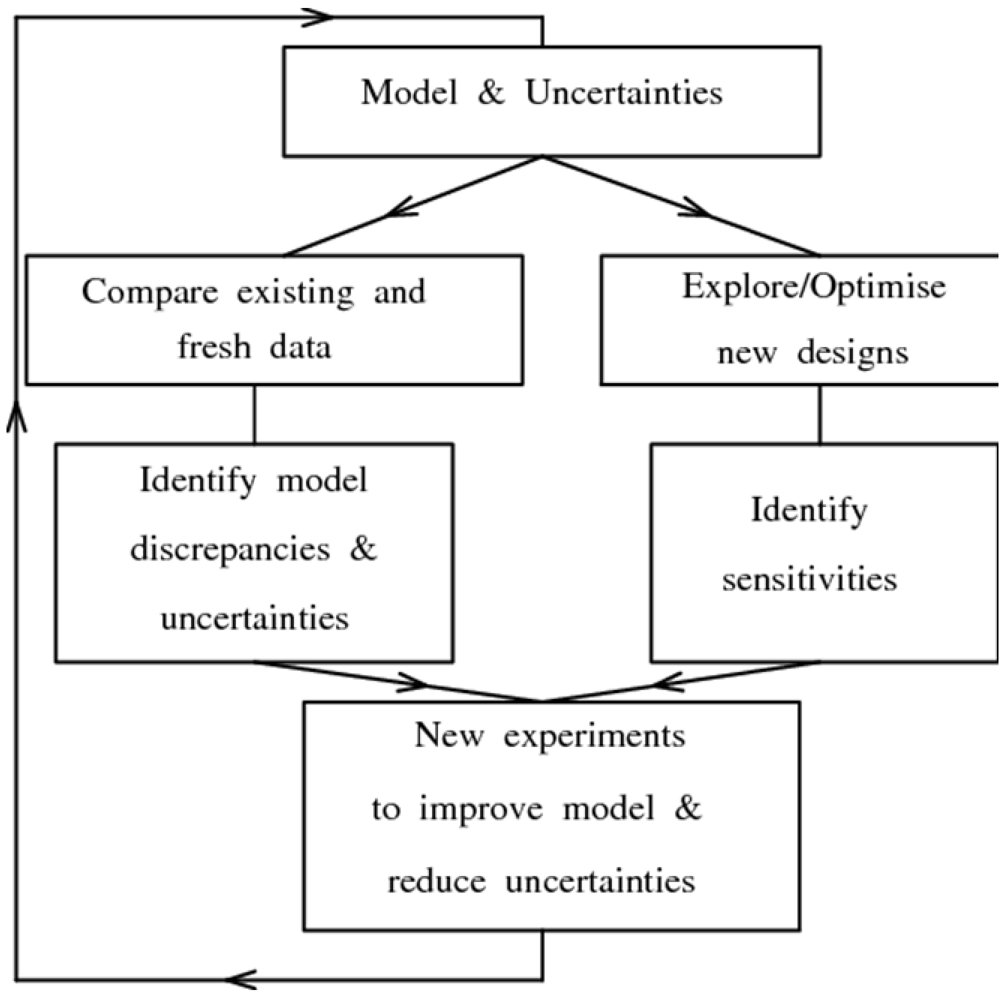
Cmdwrap directory records time, executable and data

Reactor Design Problem

Reactor Design Problem

Aims (SMITER project as microcosm):

- Predict, interpret and control operation of burning plasma experiment such as ITER.
- Design demonstration fusion reactor such as DEMO.



Modelling a Fusion Reactor

- Same issues as for any electrical power station:
  a. Fluid flow, heat transfer
  b. Mechanical stress, etc. etc.
- Large uncertainties in reactor core and nuclear data:
  - Plasma turbulence affecting
    a. Fusion yield (exponentially on T - heat transport)
    b. Power exhaust (heat leaks out to first wall)
    c. Instability (intermittency, e.g. ELMs)
  - Nuclear data cross-sections
  - Material properties under irradiation by 14MeV neutrons

Software Progression

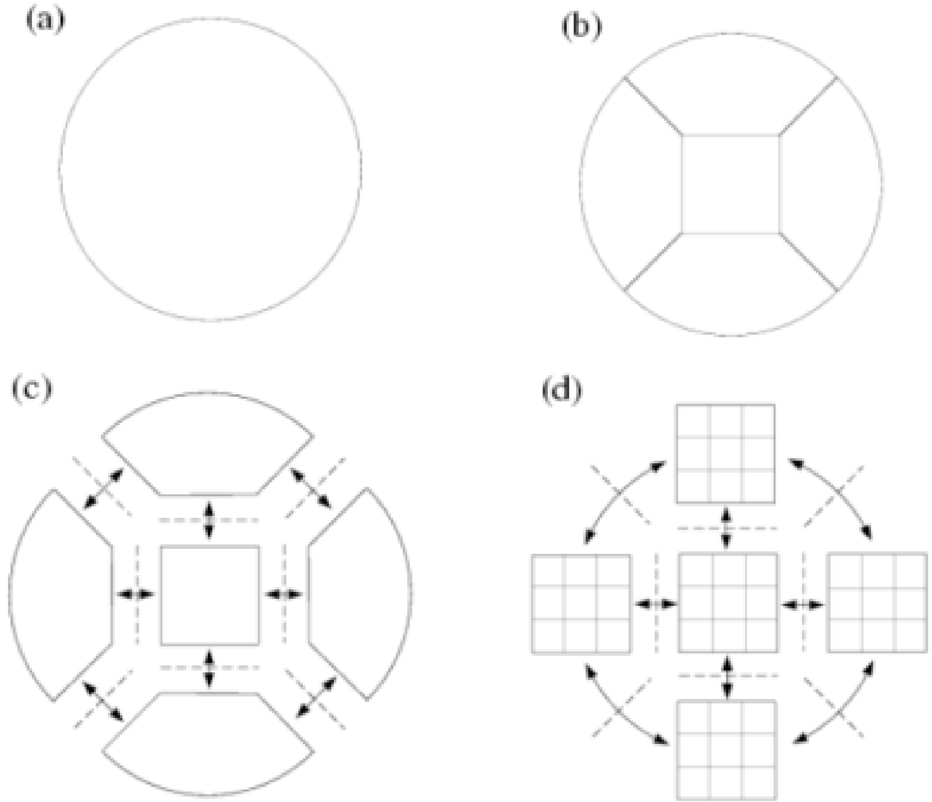
a) Power balance model (Zero-D) such as in CCFE's PROCESS code (constrained optimiser)
--------*develop*------------

b) +

c) Split into sub-problems for more detailed 1-, 2-, …,6-D modelling and define inter-relationships

d) Define objects within sub-problems

And recurse and refine over 30+ years



Guidelines for Development

- Exploit expertise of different professionals.
- Ensure software always produces an answer, always with error estimates.
- Ensure software capable of spectral accuracy.
- Redundancy in major components.
- Recommend rather than impose standards, software tools and libraries.
- Have a policy on use of OpenSource software

The Professional Matrix

Professional	*Main role*	*Main code usage*
Engineer	Design	Ensembles/Scans
Physicist	Select and define physics	Single run
Mathematician	Solvers and algorithms	Library/subprogram
Computer Scientist	Compilation and hardware	Machine Level

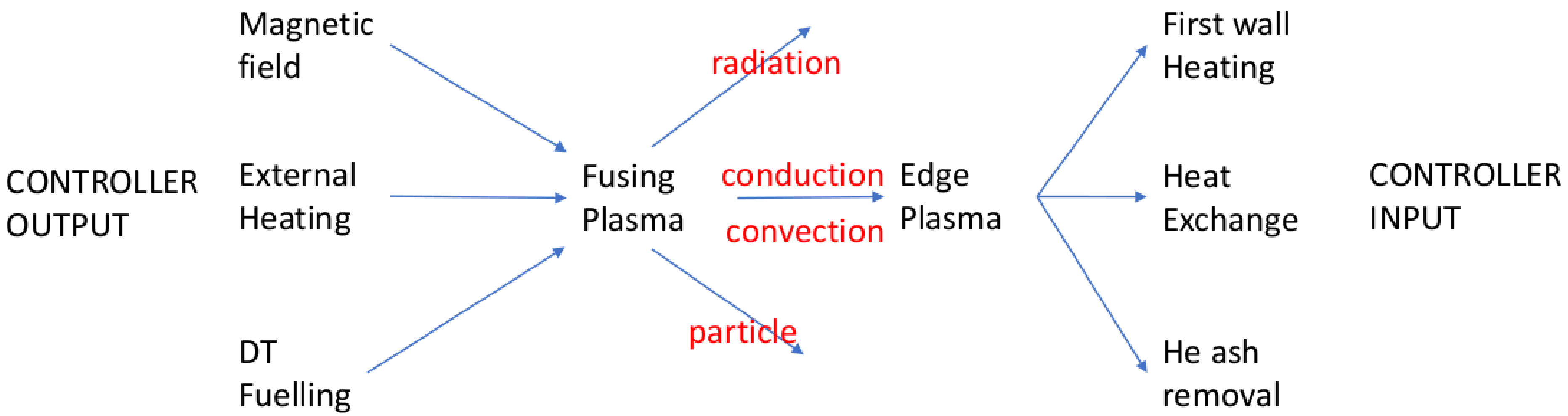
- Blurring of roles is expected

The Professional Matrix

Professional	*Main role*	*Main code usage*
Engineer (Arter)	Design	Ensembles/Scans
Physicist (Eastwood)	Select and define physics	Single run
Mathematician (Brealey)	Solvers and algorithms	Library/subprogram
Computer Scientist (Hockney)	Compilation and hardware	Machine Level

- Blurring of roles is expected (3DPIC/EMX development)

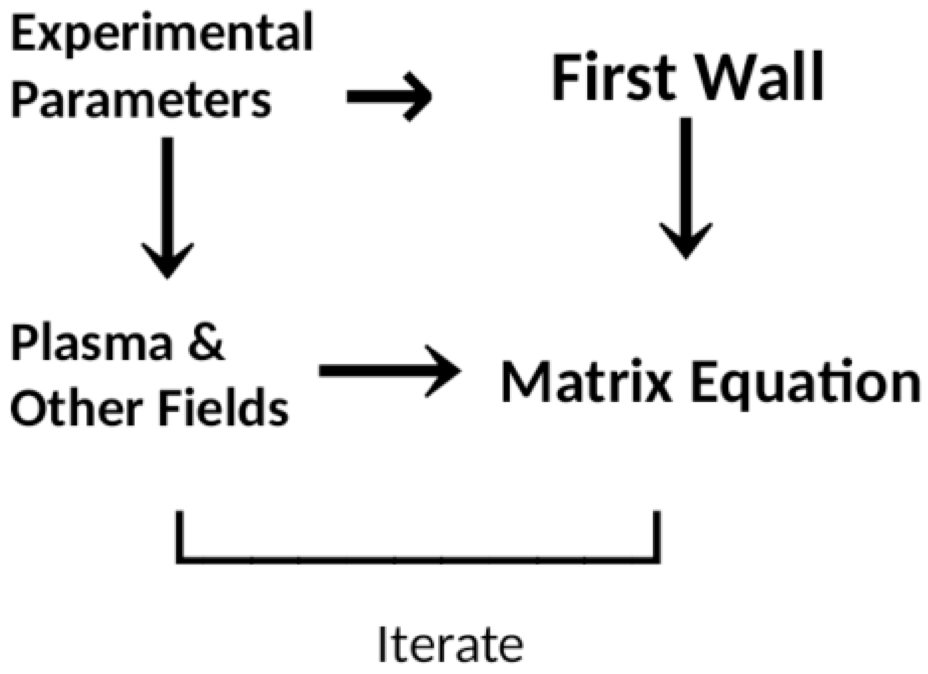
Fusion reactor dynamics



- Only subset of interrelationships shown
- Feedback from right to left to complete control loop

Close-coupled Approach

- Feedbacks and physics of energy transport demand close-coupling, via one matrix equation.
- Robustness and flexibility point to object-oriented design.
- Objects whatever their meaning must ultimately define matrix coefficients.
- Coefficient definition indirect through other matrix, particle or ray-tracing calculations



Summary

- Outlined the key modelling issues for design of fusion reactor core:
  - SMARDDA software as the microcosm.
  - Need for software capable of continuous development.
- History at Culham implies that it is possible to design software for 30 years of development.
- Guidelines for selecting a solution presented.
- Possible solution outlined.

Acknowledgements

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