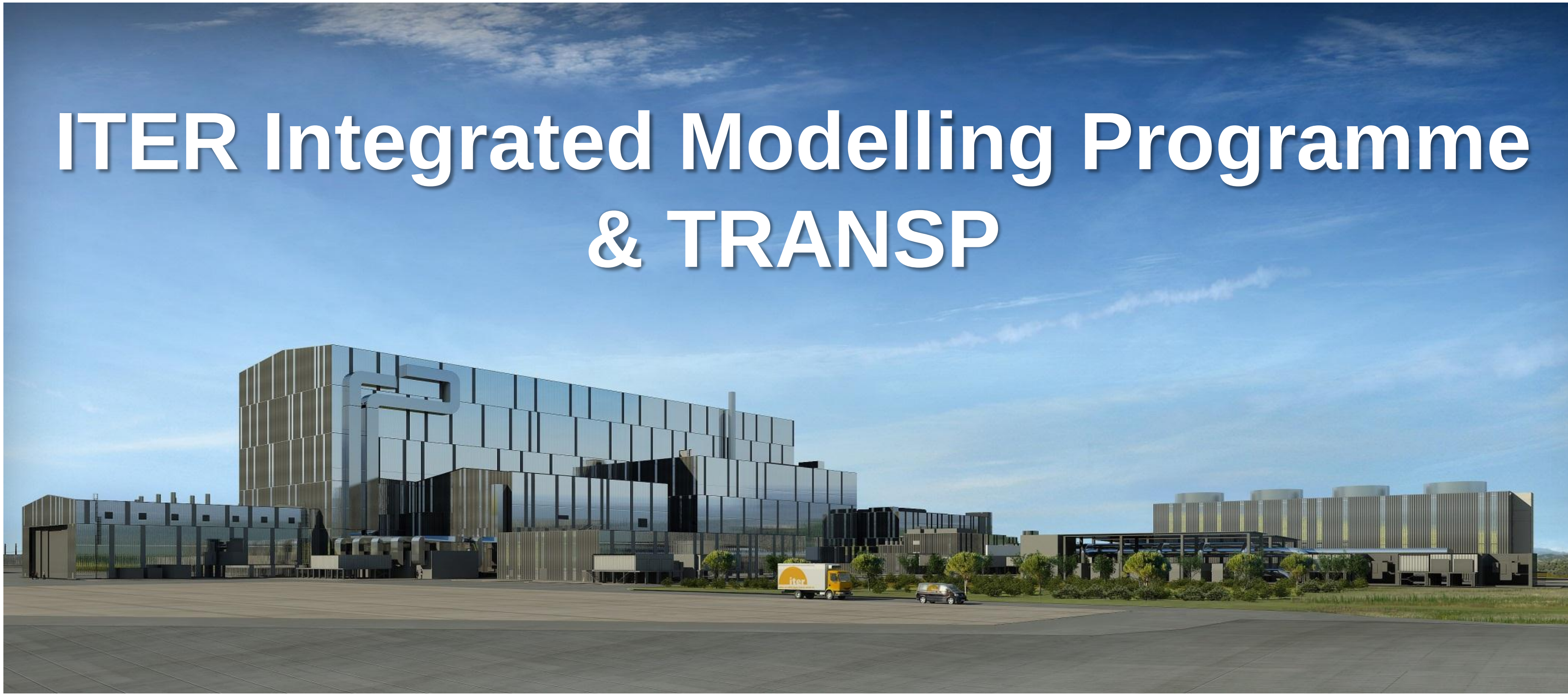
ITER Integrated Modelling Programme & TRANSP



SD Pinches

ITER Organization

The views and opinions expressed herein do not necessarily reflect those of the ITER Organization

ITER Integrated Modelling Programme

- A programme on integrated modelling and control of fusion plasmas, including benchmarking and validation activities, co-ordinated by the ITER Organization, but developed using relevant expertise within the Members' fusion programmes
- Overall aims of programme are to meet initial needs of ITER Project for more accurate predictions of ITER fusion performance and for efficient control of ITER plasmas, to support the preparation for ITER operation and, in the longer term, to provide the modelling and control tools required for the ITER exploitation phase

Endorsed by 1st ITER Council, November 2007

ITER Integrated Modelling Programme

- Scope and Purpose
  - Covers all aspects of physics modelling to aid planning and executing ITER Research Plan
  - Supports Plasma Operations and Plasma Research
  - Extensive set of “Use Cases” requiring broad spectrum of codes
  - Engages community in development
    - Close collaboration with ITER Members’ domestic fusion programmes
    - Particularly for verification and validation (cf. experimental results)
  - Ensures reproducibility and promotes longevity
    - Provenance tracking: Historical record of modelling work and results
- Implementation
  - Integrated Modelling & Analysis Suite (IMAS)
    - Based on earlier work by EU EFDA-ITM / EUROfusion-WPCD

Unwritten Design Principles

- Be pragmatic, don’t re-invent the wheel
  - Don’t have resources not to be!
- Be lightweight, flexible and objective (agile approach)
  - Don’t be biased, compare and use best available
- Be inclusive and open (not proprietary)
  - Be generic wherever possible and not specific
  - Interoperable with existing systems and data
- Make it easy for everyone to contribute
  - All improvements should be easy to include
  - Make attractive to use
- Be reproducible
  - Basis of good science
  - Provenance tracking
- Be useful!

Framework for Integrated Modelling Programme

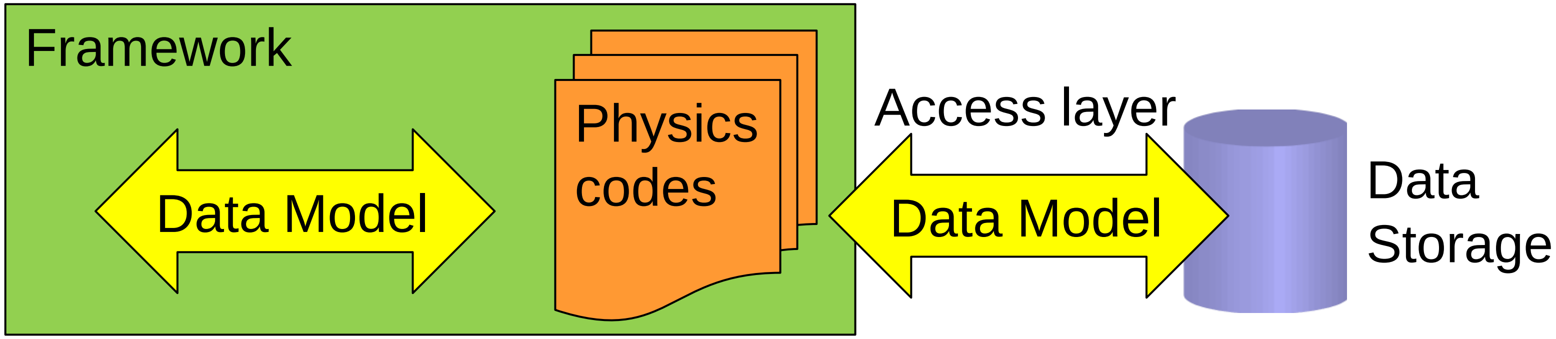
INTEGRATED MODELLING & ANALYSIS SUITE (IMAS)

Integrated Modelling & Analysis Suite (IMAS)

- Physics modelling tools to support Plasma Operations
  - Preparation of scenarios to support ITER Research Programme
  - Validation of pulses prior to operation
  - During shots for plasma reconstruction and live display
  - Post-pulse for comprehensive reconstruction using full set of diagnostic measurements
  - Components describing macroscopic behaviour should improve as ITER explores new physics domain of burning plasmas
- Tools must be computationally efficient, robust, well-documented and interface with other systems
  - Must be validated and have associated regressions tests
- Managed by IO and accessible to all ITER Members
  - Use distributed revision control system (git) to promote collaborative development
  - Revisions are automatically built and regression tested

Integrated Modelling & Analysis Suite (IMAS)

- ITER Physics Data Model
  - Applicable for all physics usages
- Physics Codes
  - To support Plasma Operations and Plasma Research
  - Contributed and validated by ITER Members
- Workflow Engine
  - To orchestrate execution of modelling workflows



ITER Physics Data Model

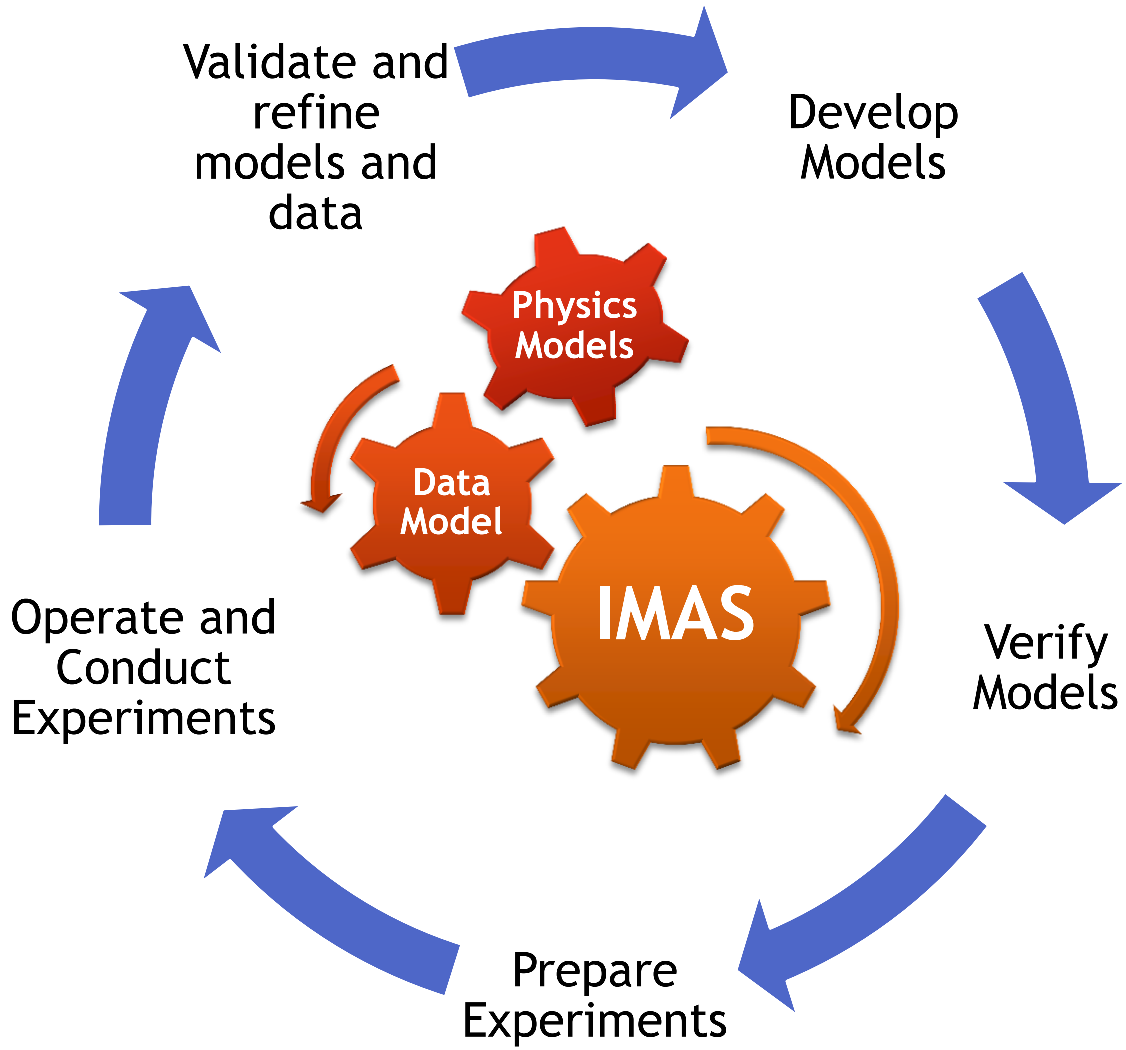
- Used for both experimental (all devices) and simulation data
- Used between physics codes and from/to storage
- Data Dictionary defines structuring and naming of data
  - Rules & Guidelines agreed following internal/external review (v3.0)
  - Uses a tree structure (allows re-use of names)
  - Automated definition of data structures for all supported languages
    - C/C++, Fortran, Java, Python, Matlab and IDL
- Interface Data Structures (IDSs)
  - Standardised entities for use between physics components
    - E.g. Diagnostic, heating system, equilibrium, core plasma profiles
  - Contains traceability (provenance) and self-description information

Data Storage

- Users write to their (~/public) directories and control access with file/directory permissions
- Remotely accessible central database will store approved data
  - Prerequisites include provenance of data producing software (SHA-1 hash of all components in software repositories) and input data

Model Development Cycle

Consolidation of physics knowledge into numerical models



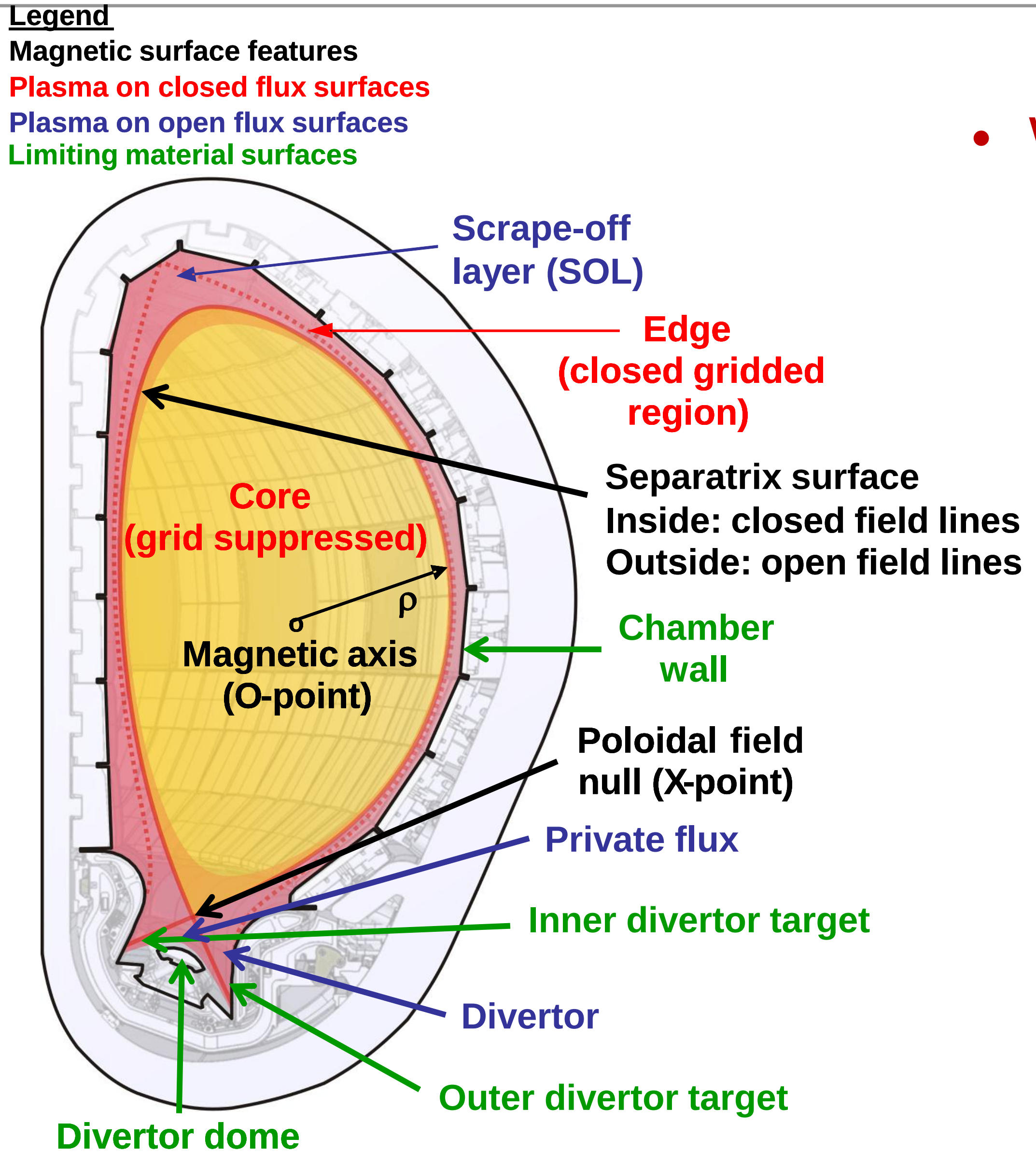
Data for Validating IMAS Workflows

- Validation is important element of IMAS development
- Validation needs data
- Data is only available on existing machines
  - IMAS needs to connect to existing (as well as future) data
- Existing experimental data stored in wide variety of formats
  - ITERDB is planned to be based upon HDF5
- IMAS needs to be able to read different storage formats
  - Members write plug-ins to read their data formats and map into Data Model in framework supported by IO (documentation, examples, etc.)
- Mapping device-specific data into Data Model needs managing
  - Data Model allowed to evolve (currently on v3.0.3)
  - Demonstrate using IDAM to manage mapping (Q2 2015)
    - For MAST and JET
  - Read (and write for storing simulation data)

IM Programme and ITPA

- **International Tokamak Physics Activity (ITPA)**
  - 7 topical groups that help address high priority R&D for ITER
- **IMAS can help support ITPA joint activities**
  - Regular presentations to ITPA Topical Groups and Coordinating Committee
- **ITPA Topical Groups are ideally placed to:**
  - Provide advice on the choice of models to integrate into IMAS to address ITER high priority R&D needs and other Use Cases
  - Help validate models and workflows through verification/benchmarking activities and against experimental data
    - ITPA TG on Energetic Particles has joint modelling activities on:
      - Calculations of NBI and ICRH fast ion distributions, $f(\mathbf{x},\mathbf{v})$
      - Benchmarking fast ion linear and nonlinear stability codes
    - ITPA TG on IOS starting joint benchmark activities on particle transport simulations and burn control simulations

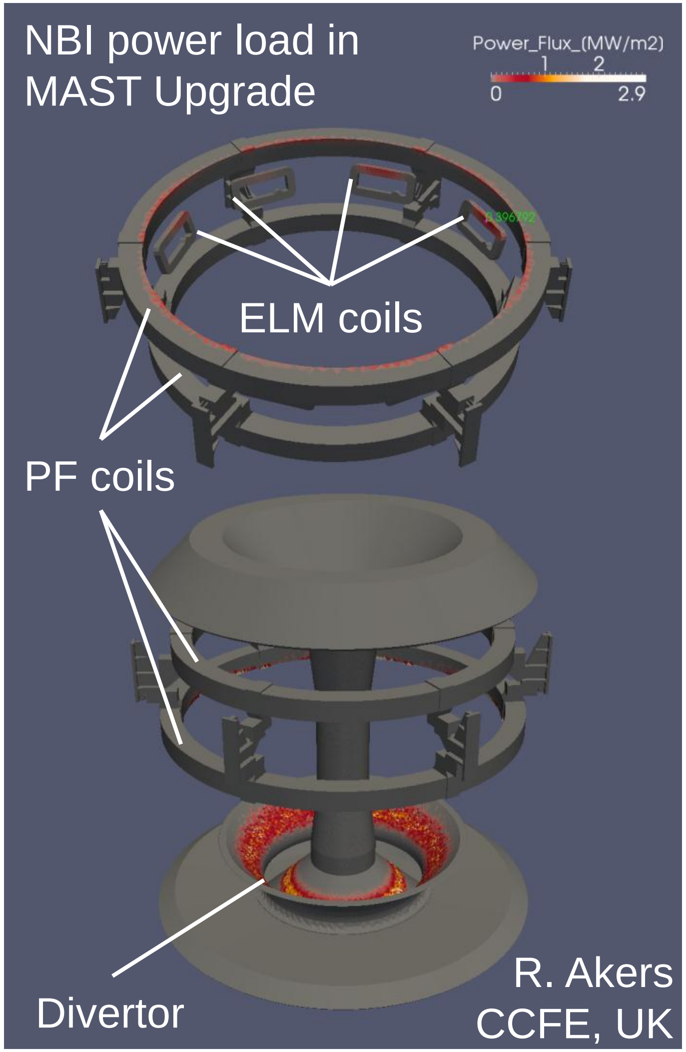
Physics Integration Challenges



- Will ultimately require:
  - Coupling of all spatial plasma domains (core, edge, scrape-off layer & divertor)
  - Dynamic coupling of individual physics models relevant to each domain
  - Interaction between plasma and PFCs
  - Coupling of plasma with external circuits, H&CD, fuelling, pumping and other systems to confine and control plasma

Computational Challenges

- Explore new algorithms and techniques as hardware evolves
  - Re-examine traditional approaches
- Exploit advances in architecture
  - E.g. Speed-up ×50 over single core by using GPU to follow fast ions → ×200 using four GPU cards
- Separate machine data from physics codes
  - Use Data Model to access machine/engineering/CAD data
    - Improved portability
- Validate physics codes towards use in engineering calculations



Computation Challenges

- Parareal technique (time parallelisation) investigated as approach to accelerate ITER transport simulations performed with CORSICA
  - 2D equilibrium package + transport models + source modules developed by Lawrence Livermore National Laboratory, USA
  - Computationally intensive
  - Parareal algorithm relies upon ability to create coarse / fine runs and the ability to restart
- With analytic source terms: Gain of **8.32** on 12 processors
- With NBI source terms: Gain of **10.13** on 32 processors

Debasmita Samaddar, ITER Monaco Postdoctoral Fellow

What will IMAS be used for?

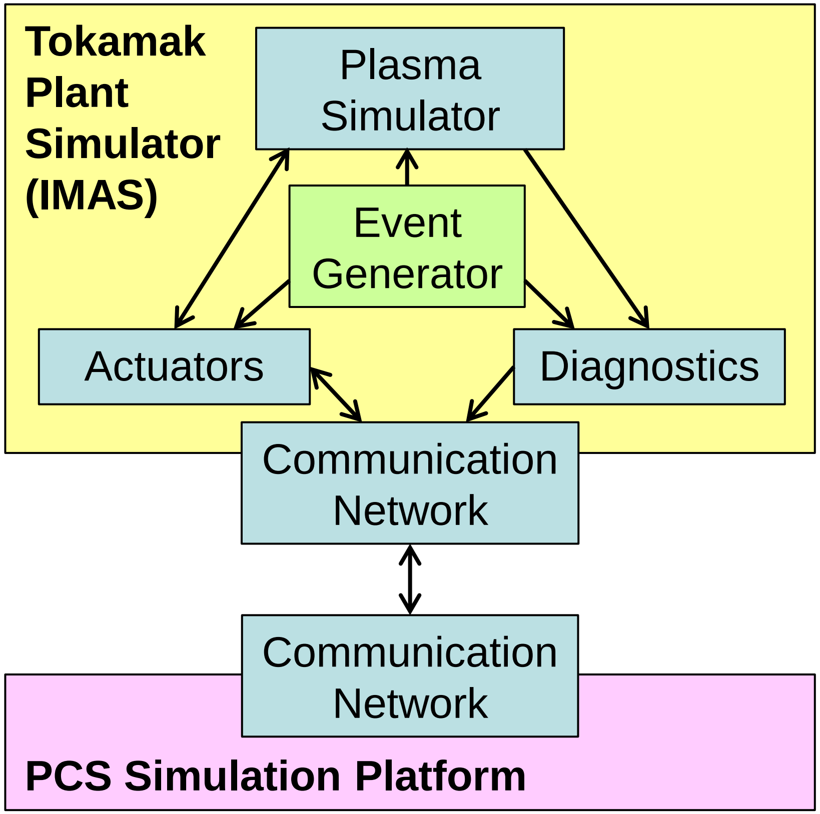
WORKFLOWS & USE CASES

Example Workflows / Use Cases

- Pulse planning/validation/execution
  - Core plasma + free boundary equilibrium + diagnostics +…
  - Live display of measurements and derived quantities
- PCS development
  - Synthetic diagnostics and combined measurements
- Plasma reconstruction
  - Including data validation, e.g. neutron rate
- Diagnostic and H&CD design, optimization and upgrade
- Ab-initio modelling of plasma phenomena
- Interpretive modelling of plasma phenomena
- Model validation and improvement, etc…

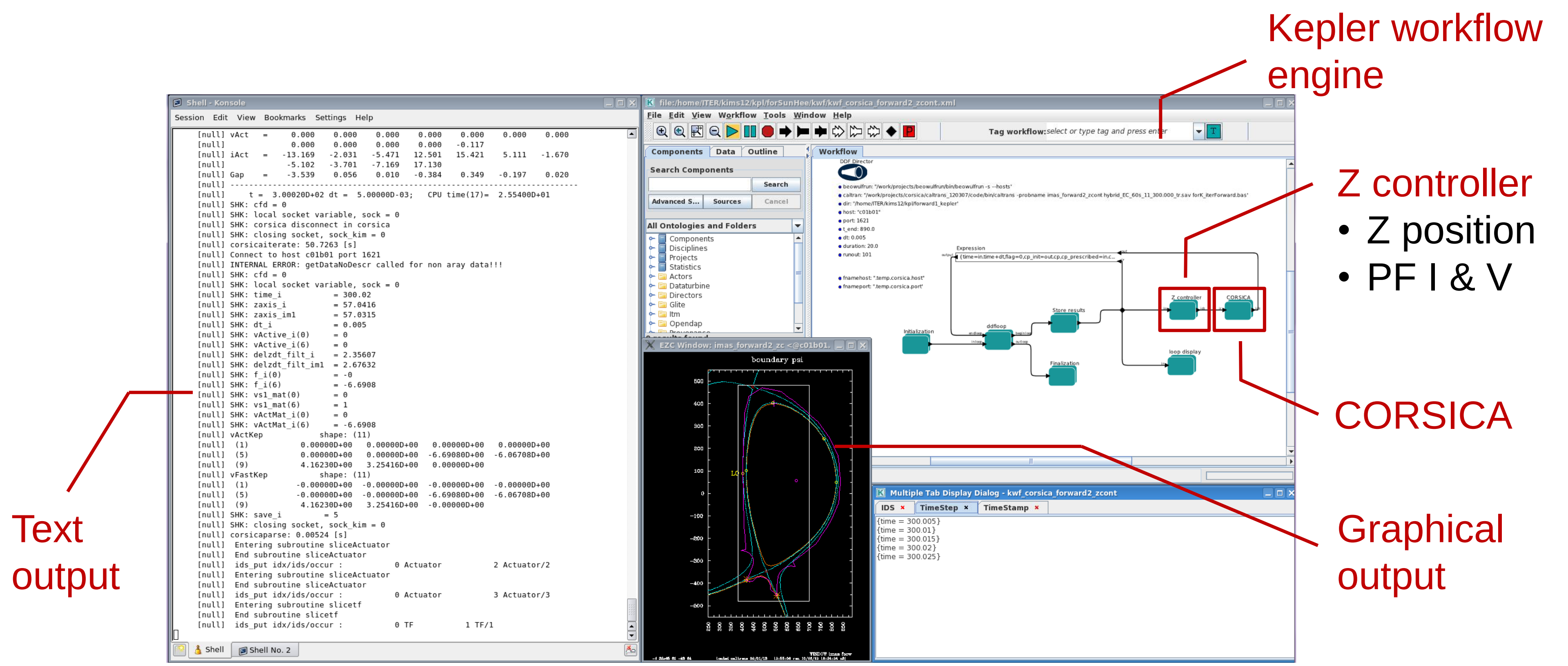
IMAS Plasma Simulator

- One of the principle applications for prototyping IM framework and developing tools required for pulse preparation
- Co-simulations of Plasma Simulator and Plasma Control System Simulation Platform
  - Basis for pulse validation
  - Develop control strategies from plasma initiation to burn control
  - Refine response to events
    - L-H transition
    - Power supply interruption
    - Diagnostic degradation / failure
  - Troubleshoot PCS during operations
  - Coupled system can guide physics model development



CORSICA-based Plasma Simulator

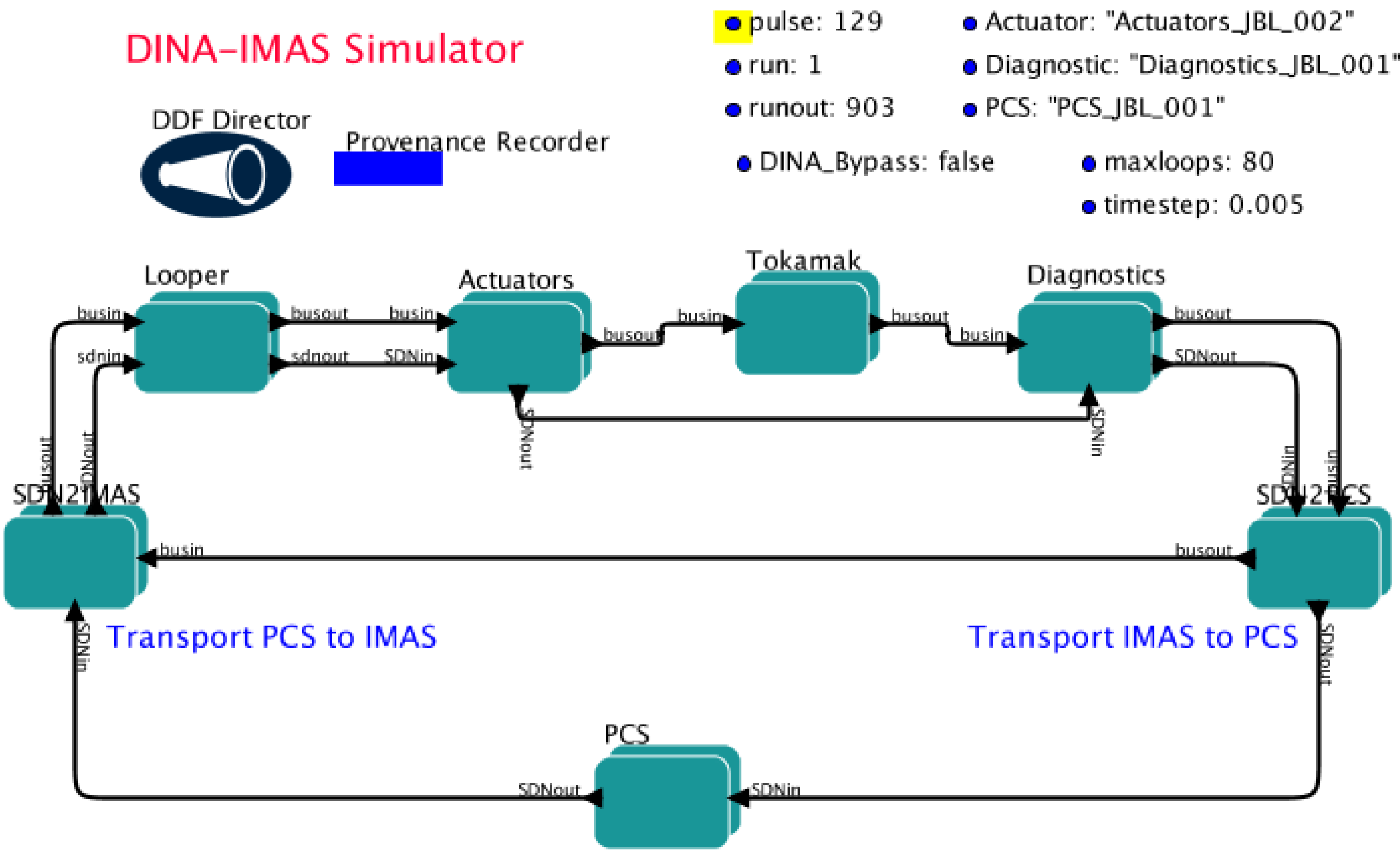
- CORSICA implemented as single workflow component
- Example: Free-boundary 12.5 MA hybrid scenario
  - Realistic sources and external vertical position (Z) controller



M Hosokawa, S H Kim, T Casper & LLNL CORSICA colleagues

DINA-based Plasma Simulator

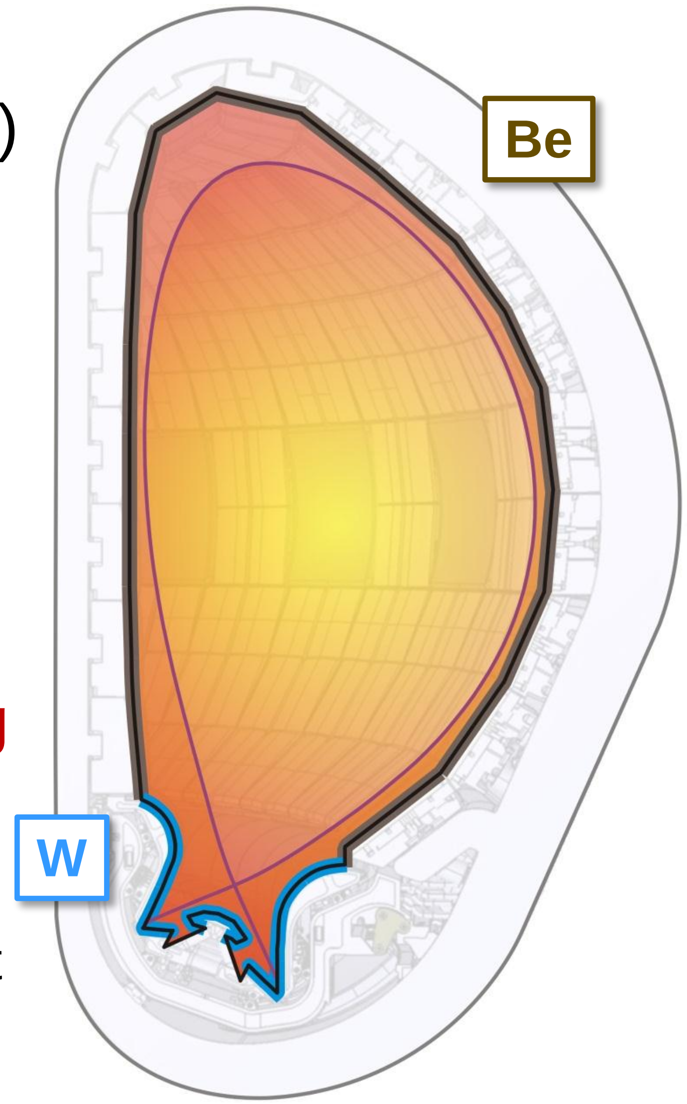
- DINA integrated into IMAS in modular fashion



J Lister, V Lukash, R Khayrutdinov and DINA colleagues

SOLPS: Scrape-Off Layer Plasma Simulation

- Primary tool for ITER divertor design
- New version: SOLPS-ITER (April 2015)
  - Aims to be new standard version used by all ITER Members (works for all devices)
  - 2D fluid plasma solver (B2.5)
  - Kinetic neutral transport solver (Eirene)
- Will be adapted to use:
  - EDGE IDS, Generalised Grid Description (GGD), Machine Description, AMNS tools
- Coupled to modules describing heating of Plasma Facing Components (PFCs)
- Coupled to core transport codes
  - ASTRA (Automated System for TRansport Analysis)
  - ETS (European Transport Solver)



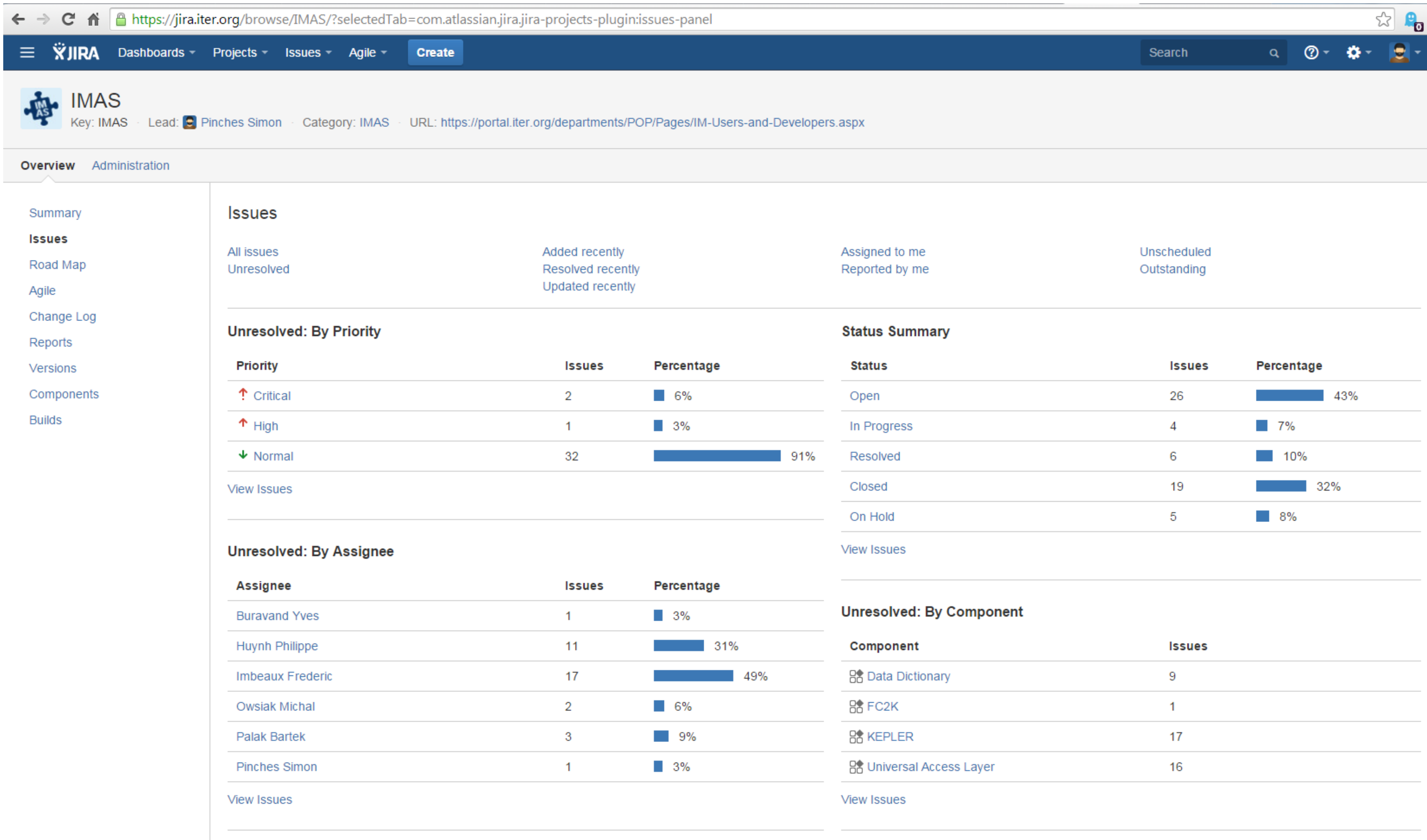
How do we manage all the elements of IMAS?

COMPONENT MANAGEMENT

Issue Tracking

- Categorised issue tracking using JIRA
  - Collaboration, support and discussion
- Project management (agile approach)
  - Follows development cycle
- Can link issues with
  - Other issues (sub-issues, tree structures, …)
  - Software development branches
  - Build and Test results

Issue Tracking



https://jira.iter.org/browse/IMAS/?selectedTab=com.atlassian.jira.jira-projects-plugin:issues-panel

JIRA Dashboards Projects Issues Agile Create Search

IMAS

Key: IMAS · Lead: Pinches Simon · Category: IMAS · URL: https://portal.iter.org/departments/POP/Pages/IM-Users-and-Developers.aspx

Overview Administration

- Summary
- Issues
- Road Map
- Agile
- Change Log
- Reports
- Versions
- Components
- Builds

Issues

All issues
Unresolved
Added recently
Resolved recently
Updated recently
Assigned to me
Reported by me
Unscheduled
Outstanding

Unresolved: By Priority

Priority	Issues	Percentage
Critical	2	6%
High	1	3%
Normal	32	91%

View Issues

Status Summary

Status	Issues	Percentage
Open	26	43%
In Progress	4	7%
Resolved	6	10%
Closed	19	32%
On Hold	5	8%

View Issues

Unresolved: By Assignee

Assignee	Issues	Percentage
Buravand Yves	1	3%
Huynh Philippe	11	31%
Imbeaux Frederic	17	49%
Owsiak Michal	2	6%
Palak Bartek	3	9%
Pinches Simon	1	3%

View Issues

Unresolved: By Component

Component	Issues
Data Dictionary	9
FC2K	1
KEPLER	17
Universal Access Layer	16

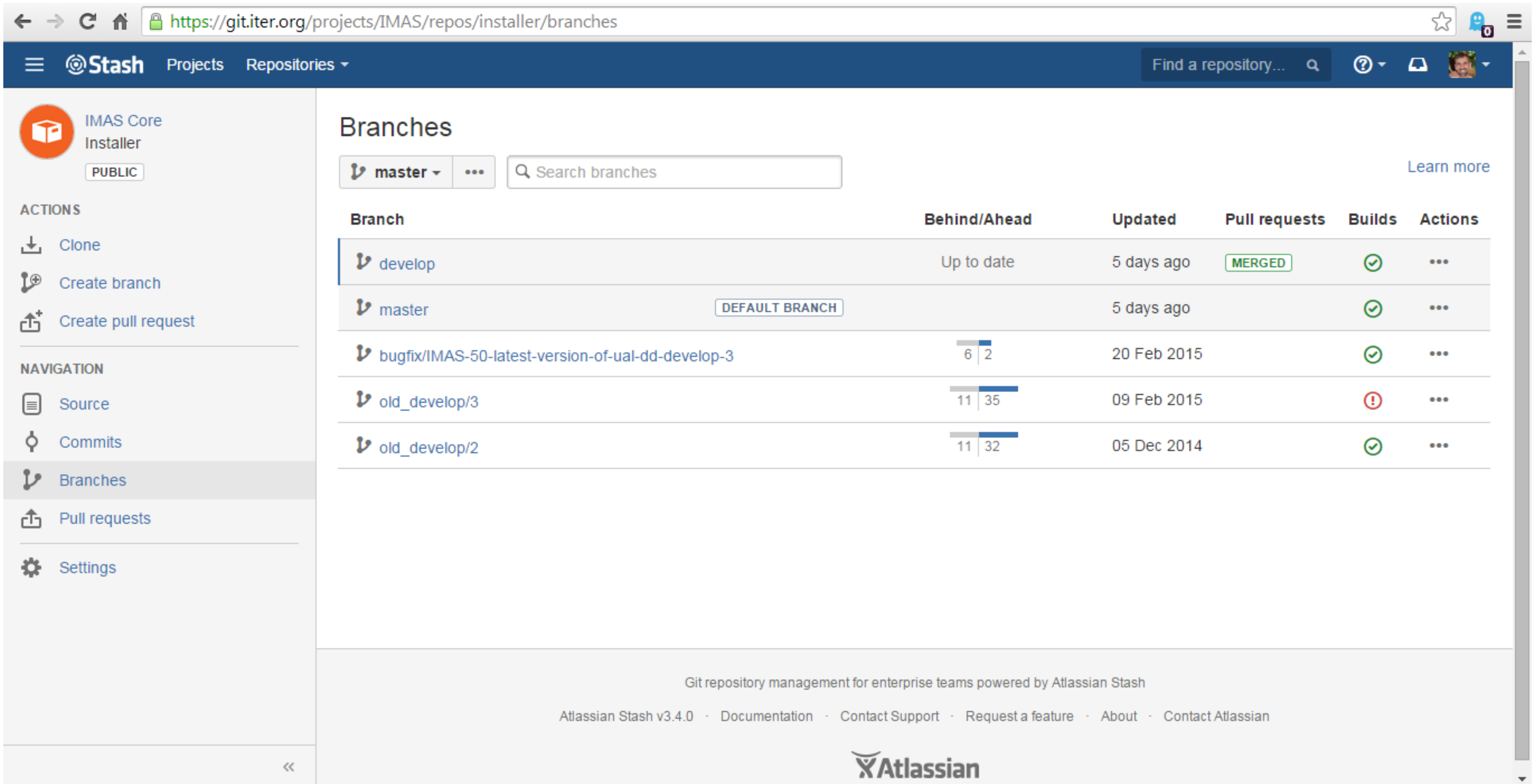
View Issues

https://jira.iter.org/browse/IMAS

Distribution Revision Control

- Why git?
  - Allows simple asynchronous concurrent distributed development
  - Allows cheap branching and easy merging
- IMAS has adopted a branch-based development workflow
  - Focussed on bringing contributions together (i.e. limit forking)
  - Branch-based access controls
  - Can enforce code review and successful build/test before being merged
- Web-based graphical front-end, Stash
  - Commits can be linked to JIRA issues
  - Commits trigger building and testing on continuous integration server, Bamboo
- Can be used in conjunction with other revision control systems
  - E.g. Subversion, CVS and Mercurial
  - Leads to some loss of workflow flexibility

Distribution Revision Control



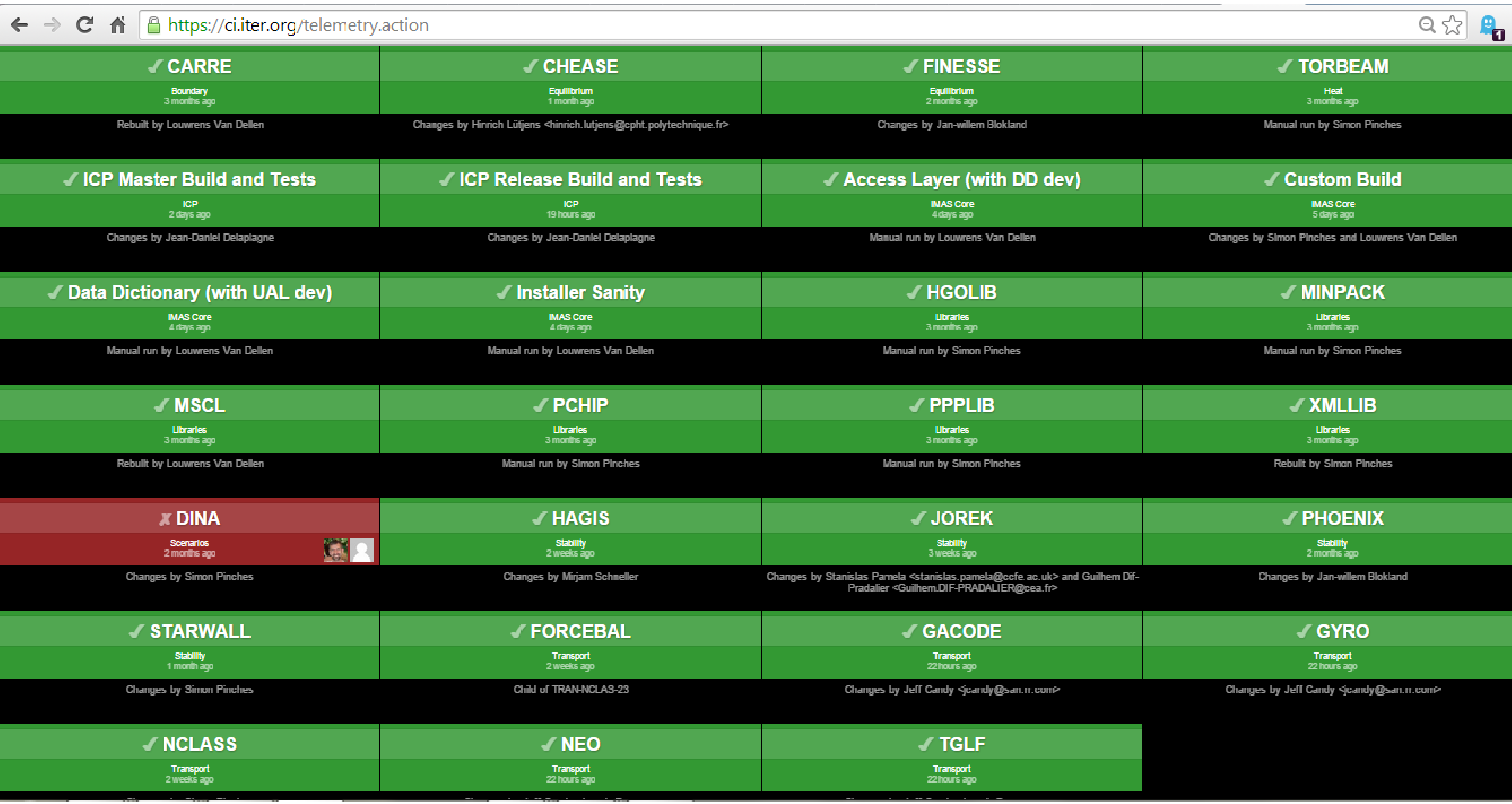
https://git.iter.org

Continuous Integration Server

- Automatic build of components
  - Triggered as commits are pushed to repository
- Automatic regression testing of components
  - Branch class determines test
  - Can depend upon other components and elements of IMAS
- Automatic deployment
  - Of components and documentation
- Reporting

Bamboo

Auto-Builds / Regression Tests



https://ci.iter.org/telemetry.action

Bamboo

Code	Project	Contact	Affiliation	Member	Licence	Revision Control	Auto-Build	Regression Tests	Data Model
CHEASE	EQ	Olivier Sauter	CRPP	EU	1	1	1		3
NCLASS	TRANS	Par Strand	Chalmers	EU	1	1	1		3
CORSICA	SCEN	Lynda LoDestro	LLNL	US		1			3
DINA	SCEN	Sergei Konovalov	Kurchatov	RF	1	1	1		2
GYRO	TRANS	Jeff Candy	GA	US	1	1	1	1	
NEO	TRANS	Emily Belli	GA	US	1	1	1	1	
TGLF	TRANS	Jeff Candy	GA	US	1	1	1	1	
FINESSE	EQ	Jan-Willem Blokland	DIFFER	EU	1	1	1		
HAGIS	STAB	Simon Pinches	IO	IO	1	1	1		
PHOENIX	STAB	Jan-Willem Blokland	DIFFER	EU	1	1	1		
TORIC	HEAT	Roberto Bilato	IPP	EU	1	1	1		
CARRE	BND	David Coster	IPP	EU		1	1		
JOREK	STAB	Guido Huijsmans	IO	IO		1	1		
TORBEAM	HEAT	Emanuele Poli	IPP	EU		1	1		
DIVGEO	BND	Andre Kukushkin	IO	IO	1	1			
EIRENE	BND	Detlev Reiter	FZJ	EU	1	1			
HELENA	EQ	Guido Huijsmans	IO	IO	1	1			
SOLPS4.3	BND	Andre Kukushkin	Kurchatov	RF	1	1			
ASTRA	SCEN	Emiliano Fable	IPP	EU		1			
B2.5	BND	Bas Braams	IAEA	EU		1			
EFIT++	EQ	Lynton Appel	CCFE	EU		1			
NEMO	HEAT	Mireille Schneider	CEA	EU		1			
RISK	HEAT	Mireille Schneider	CEA	EU		1			
SOLPS-ITER	BND	Xavier Bonnin	IO	IO		1			
SPOT	HEAT	Mireille Schneider	CEA	EU		1			
BOUT++	SCEN	Ben Dudsen	Uni. of York	EU	1				
ETS-C	SCEN	Frederic Imbeaux	CEA	EU	1				
GKW	TRANS	Arthur Peeters	Uni. Bayreuth	EU	1				
PARASOL	BND	Shunsuke Ide	JAEA	JA	1				
TASK	SCEN	Atsushi Fukuyama	Kyoto Uni.	JA	1				
ASCOT	TRAJ	Tania Kurki-Suonio	Aalto	EU					
CEDRES++	EQ	Eric Nardon	CEA	EU					
ETS-A	SCEN	Denis Kalupin	EUROfusion	EU					
HCDTOOLS	HEAT	Thomas Johnson	KTH	EU					
JINTRAC	SCEN	Michele Romanelli	CCFE	EU					
LOCUST	TRAJ	Rob Akers	CCFE	EU					
MARS-[F/K/Q]	STAB	Yueqiang Liu	CCFE	EU					
OFMC	TRAJ	Toshihiro Oikawa	IO	IO					
RFOF	HEAT	Thomas Johnson	KTH	EU					
TRANSP	SCEN	Stan Kaye	PPPL	US					

Status and Outlook for ITER IM Programme

- Maturing IMAS framework available on ITER's HPC cluster
  - Physics Data Model sufficient for majority of initial workflows
  - First workflows based on integrating ITER's existing physics codes
  - Increasing interest to incorporate and adapt physics components
  - Software management tools: Issue tracking, revision control (Git) and auto-building/regression testing available for all components
- Future developments
  - Integrate and adapt physics components to extend physics capabilities
  - Continue to extend Data Model compliant with Rules & Guidelines
  - Continue to support remote use by beta testers
    - 79 people from within ITER Members trained in use of IMAS this year
  - Modularise existing workflows and extend physics capabilities
  - Package framework for local use, testing and validation within ITER Members' domestic fusion programmes

Local Installation of IMAS

- To support adaptation of codes to IMAS
  - Available Q2 2015, but no need to wait
  - IMAS is available on ITER's HPC cluster now
- Validation of IMAS and workflows easier in a familiar computing environment
  - Eliminate need to work remotely (if this is a problem)
- Any local developments can easily be incorporated into future releases of IMAS
  - Software management infrastructure used for complete IMAS framework (including installation tools) and physics components

Next Steps for IMAS (2015)

- Implement a Plasma Simulator as a modular physics workflow demonstrating the capabilities and approach of IMAS that can be used as a template for the development of other workflows
  - Kepler workflow based on European Transport Solver (ETS) and using CHEASE (for equilibrum), NCLASS (for neoclassical transport), etc.
- Extend Data Model to treat error bars
  - Dynamic handled in Access Layer
- Create Machine Descriptions
- Extend data access capabilities to provide access to existing (and future!) experimental data in form of IDSs

Possible steps for integration of TRANSP into IMAS

- Licence TRANSP for use within IMAS
- TRANSP installation and compilation at ITER
  - Host TRANSP in ITER git repositories
    - Can link to TRANSP svn repository (as trusted host)
- Adapt TRANSP to use ITER Data Model for overall I/O
- Adapt TRANSP to exchange data with other physics components using ITER Data Model during simulation
- Create modular TRANSP workflow within IMAS by creating components that exchange data using ITER Data Model
  - Allows flexible use of other IMAS physics components within TRANSP workflow

ITER's Modelling Needs

- Need predictive code for simulations of ITER scenarios
  - Complete pulse from breakdown to termination
  - Respecting plant limitations (e.g. PF circuits)
  - Free-boundary evolution including realistic plasma transport
    - With multiple impurities (W, Be, He, Ne, Ar, N,…)
  - Extensible to include edge/SOL & PFCs
  - Modular inclusion of sources: H&CD, fuelling (pellets & gas)
  - Description of transients: H-L/L-H, MHD (sawteeth, ELMs, AE)
- All components must be
  - Well documented (users and developers) with training
  - Easy to maintain / supported as/when required
  - Modular, extensible, flexible, distributable
  - Hosted at ITER and adapted to IMAS (principally Data Model)
  - Rigorously tested and validated with regression tests (CI server)
  - Match requirements for Use Cases (physics and performance)

More Information

- ITER Integrated Modelling Programme (2EFR4K)
  – https://user.iter.org/?uid=2EFR4K&action=get_document
- Links to training material, data model and software management tools (repositories, issue tracking and auto-building/regression testing/continuous integration)
  – https://portal.iter.org/departments/POP/Pages/IM-Users-and-Developers.aspx