U.S. PFC-related computer codes: a survey*

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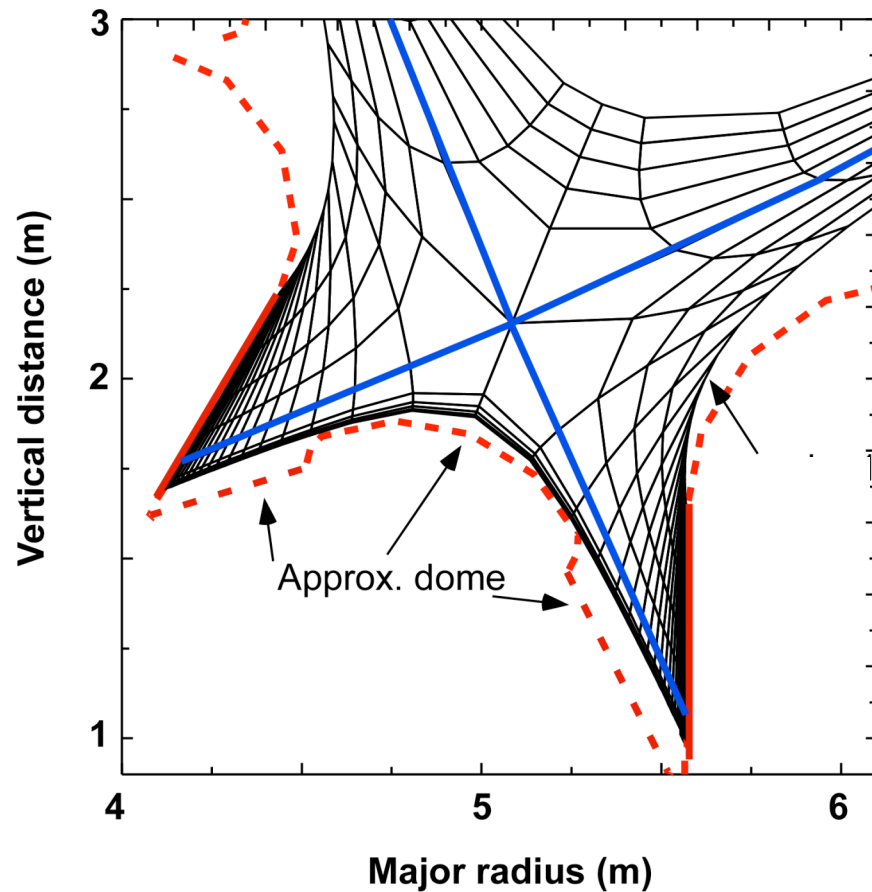
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and many PFC community participants

PFC codes must simulate a wide variety of physical processes and components

ITER divertor region illustrates related issues

Approx. dome

PFC codes must simulate a wide variety of physical processes and components

ITER divertor region illustrates related issues

- **Edge plasmas and neutrals (transport, turbulence)**

- **Magnetic field …**

- **Near-surface plasma/neutrals**

- **Sputtering, redep., recycling, sheaths …**

- **Material structure (MD); evolution**

- **Thermal and stress analysis …**
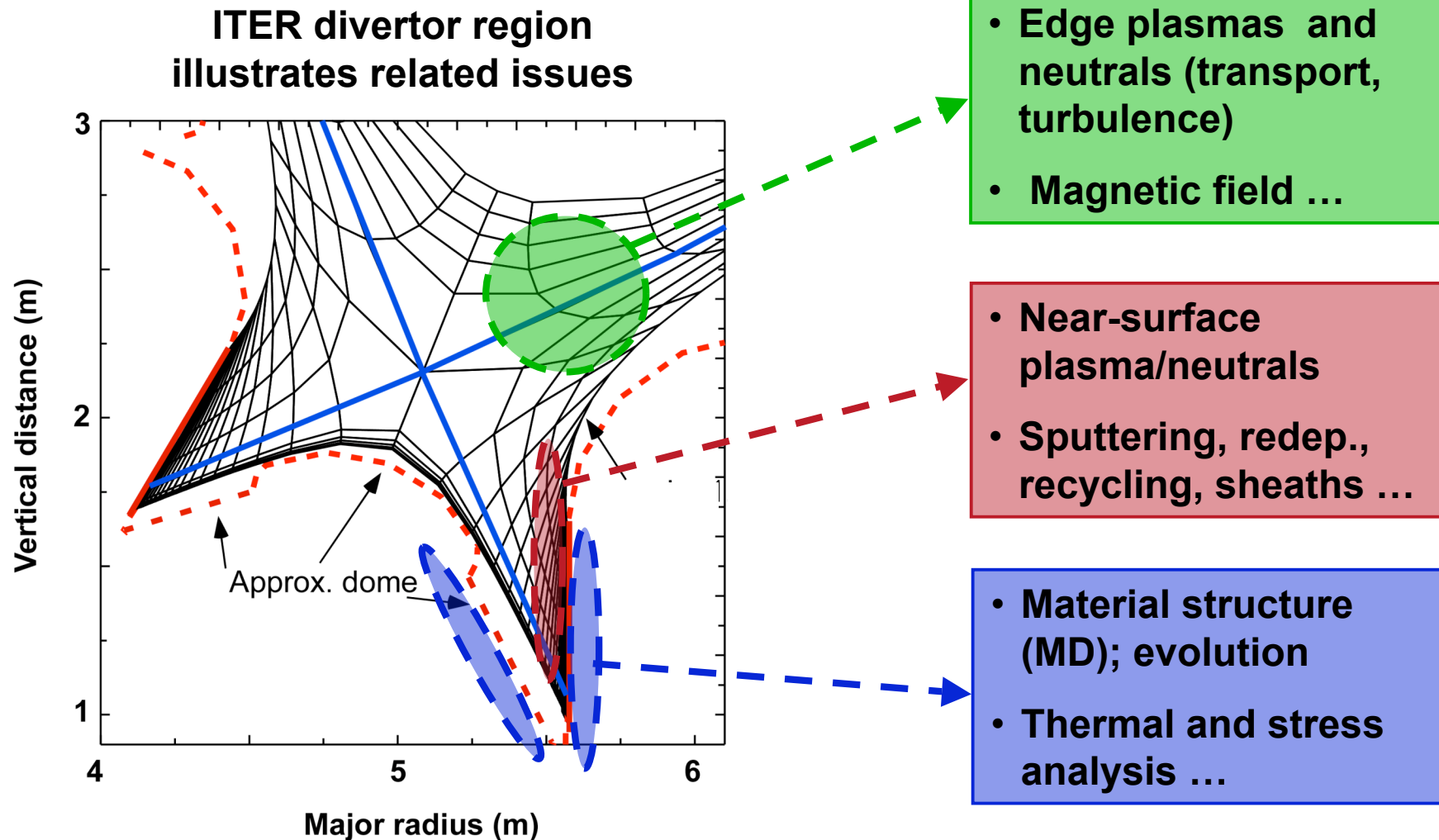
PFC researchers answered the following questions:

- **Abstract: description, authors**

- **References:published, reports**

- **Physical problem being simulated:**

- **Space and time domain: 1-3 D, transient, steady-state**

- **Underlying physics equations and processes included:**

- **Numerical models:**

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- **Underlying physics equations and processes included:**

- **Numerical models:**

- **Computer science and numerical algorithms:**

- **Computer requirements; performance:**

- **Verification and validation:**

- **Interaction with other codes:**

- **User community:**

Plasma and neutral codes for the edge region

- **KINETIC TRANSPORT CODES**
  - **REDEP-WBC:** 3D,3v Monte Carlo ions, neutrals, Coulomb collisions with background, sputtering and redeposition, Brooks, ANL
  - **BPHI-3D:** 3D,3v, steady-state, PIC ions, Boltzmann electrons, sheath formation, Brooks, ANL
  - **MCI:** 3D, 2v, Monte Carlo ions, neutrals, Coulomb collisions with background, sputtering and transport in full SOL, Evans, GA
  - **DEGAS2:** 3D,3v, Monte Carlo neutrals in realistic geometry, Stotler, PPPL
  - **DUSTT:** 3D,3v, Monte Carlo dust particles in plasma edge, neutral and ionized, Pigarov, UCSD

- **FLUID TRANSPORT CODES**
  - **UEDGE:** 2D, plasma/neutral fluids (occasional MC), impurities, radiation via implicit finite volume, Rognlien, LLNL
  - **B2.5:** 2D, plasma fluids, neutral fluid or MC, impurities, radiation via finite volume, used by Owen, ORNL
  - **HKH:** 1D, SOL plasma properties from fluid model, radiation, from Harrison, Kukushkin, used by Ulrickson, SNL

- **INTEGRATED PACKAGES**
  - **HEIGHTS:** 1D-3D, combines plasma transport, radiation, and PMI in various approx., Hassanein, ANL

- **PLASMA TURBULENCE CODES**
  - **BOUT:** 3D, plasma fluid model in full tokamak geometry, provides plasma turbulence fluxes to walls, Xu, Umansky, LLNL

PFC material-surface physics includes MD, BCA, and liquid MHD

- **MOLECULAR DYNAMICS**
  - **MolDyn:** 3D, 3v, Newton eqns for many-body Brenner potentials, Alman, UIUC
  - **MDCASK:** 3D, 3v, Newton eqns. for many-body Brenner and AIREBO potentials, radiation, surface evolution, Bringa, Gilmer LLNL
  - **"MDLS:"** 3D, 3v, Newton eqns. for many-body potentials, Li, H, He, Insepov, ANL

- **BINARY COLLISION APPROX. (BCA)**
  - **ITMC:** 3D, 3v?, Monte Carlo ion interaction with materials, includes Coulomb collisions, atomic potentials, (BCA?), Hassanein, ANL
  - **VFTRIM-3D:** 3D, 3v, Monte Carlo particles interaction with materials, BCA model, includes rough-surface effects, Shaheen, UIUC

- **HYBRID MD/BCA**
  - **MD-TRIM-3D:** 3D, 3v, combines Monte Carlo andMD many-body effects for sputtering, etc., Allain, ANL, Ruzic, UIUC

- **LIQUID-FLOW ANALYSIS**
  - **HIMAG:** 1D-3D, Navier-Stokes fluid with MHD via finite difference, liquid flow, Munipalli, HyPerComp
  - **MetaFlow:** 1D-3D, fluid equations with MHD via lattice Boltzmann, liquid flow, may be applicable to edge plasmas, Pattison, MetaHeuristics

PFC material structures use a wide range of codes for analysis and design

- **STRESS, HEAT, AND CAD**
  - **CUBIT:** 3D, mesh generation code for finite elements, SNL
  - **FILM-30:** 1D, heat transfer at solid-to-water boundary, SNL
  - **PFCHF:** 2D, cylindrical, maps B-field lines to surfaces for PFC heat flux, Ulrickson, SNL
  - **HEAT-1D:** 1D, time, thermal transport in PFC from plasma heat flux, Ulrickson, SNL
  - **IHC:** 1D, time, material heat conduction with temperature dependent properties, Ulrickson, SNL
  - **NdotB:** 3D, maps plasma heat flux to PFCs, Ulrickson, SNL
  - **TMAP7:** 1D, transport of tritium and other gas in materials via diffusion model, Longhurst, INNEL

- **STRESS, HEAT, AND CAD - commercial**
  - **ABAQUS:** 2D and 3D, finite element stress and heat transfer, commercial code used by SNL
  - **CATIA:** 3D, CAD package, commercial code used by SNL
  - **PATRAN:** 3D?, CAE package for PFC configuration, used as input for ABAQUS analysis, commercial code used by SNL
  - **CFD 2000:** 2D and 3D, Navier-Stokes fluid eqns., commercial code used by SNL
  - **OPERA:** 2D, 3D, finite element solution to Maxwell's eqns. in materials, commercial code used by SNL

The information gathered can be used to facilitate future work

- **Detailed information will be available on ALPS/PFC website**

- **Allows people to find codes, expertise**

- **Encourages systematic verification (solves the equations) and validation (describes reality - experiments)**

  - ITPA groups (especially Divertor and Pedestal) are pushing V&V
  - Edge Coordinating Committee is focusing on V&V
  - Growing recognition that the Fusion Community needs to put high priority on V&V