



2028-20

Joint ICTP/IAEA Workshop on Atomic and Molecular Data for Fusion

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HOW/WHY - Can we tend the fire?

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Can we tend the fire?

Three lectures course on plasma surface interaction and edge physics

III.) WHY ? Understanding plasma surface interaction

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Thanks to: V. Kotov, P. Börner



Forschungszentrum Jülich in der Helmholtz-Gemeinschaft pril 2009



Joint ICTP-IAEA Workshop on Atomic and Molecular Data for Fusion, Trieste 20-30 April 2009



Computational Science Workflow "Waterfall Model" (1960-th...) (the dream of code development managers)



Computational Science and Engineering is moving from "few effects" codes developed by small teams (1-3 scientists) to "many effect codes" codes developed by larger teams (10-20 or more).

The reality in large scale code development projects





The EU 100 TF HPC-FF will start operation in spring 2009





anostructure

ectronic structure

10nm

olecular structure

Distance

1 micron

Materials

100nm

me

Ouantur

1nm

Seconds

Microseconds

Nanoseconds

Picoseconds

Femtoseconds



2.5

Supercomputer for Fusion Science @ Jülich



Institute for Advanced Simulation Jülich Supercomputing Centre (JSC)

Present Supercomputer Environment FZJ

General Purpose Supercomputer



JUMP, 1312 processor Regatta p690+,

High Scalable Supercomputer



No. 2 in Top500-List Nov. 2007

On-line Storage, 1 PByte



Robot Silo, 4 PByte



Jülich Supercomputing Centre (JSC)



Provide sufficient convection without accumulating tritium and with sufficiently long divertor lifetime (availability).



Engineering parameter : $S_{puff} \sim (1...13) \cdot 10^{22} \text{ s}^{-1}$

core plasma

Typical Time Scales in a next step experiment with B = 10 T, R = 2 m, $n_e = 10^{14}$ cm⁻³, T = 10 keV



Fusion Simulation Project Vol.2, FESAC ISOFS Subcommittee Final Report, Dec. 2002

Core plasma Well separated: transport – turbulence: good !

Typical Time Scales in a next step experiment with B = 10 T, R = 2 m, $n_e = 10^{14}$ cm⁻³, T = 10 keV



EDGE plasma

- No clearly separated timescales, i.e. no natural separation into reduced sub-models.
- Far more challenging than at inito core plasma transport: There turbulence and transport time scales are clearly separable.
- Similar situation: Computational material and PWI science



Thanks to: R.Schneider, IPP Greifswald

Generic kinetic (transport) equation (L. Boltzmann, ~1870)

for particles travelling in a background (plasma) between collisions
with (ions) or without (neutrals) forces (Lorentz) acting on them between collisions

Basic dependent quantity: distribution function $f(\vec{r}, \vec{v}, t)$

$$\frac{\partial f(E,\vec{\Omega})}{\partial t} + v\vec{\Omega} \cdot \nabla f(E,\vec{\Omega}) + Forces = S(E,\vec{\Omega}) - v\sigma_a(E)f(E,\vec{\Omega})$$

Free flight External source Absorption

$$+ \int_{0}^{\infty} dE' \int_{4\pi} d\vec{\Omega}' \Big[v'\sigma_s \Big(E' \to E, \vec{\Omega}' \cdot \vec{\Omega} \Big) f(E',\vec{\Omega}') - v\sigma_s \Big(E \to E', \vec{\Omega} \cdot \vec{\Omega}' \Big) f(E,\vec{\Omega}) \Big]$$

Collisions, boundary conditions

Characteristics (=Trajectories) of kinetic transport equation here: MAST, Culham, UK

* CMOD (OSM-EIRENE INTERFACE) TEMPLATE



EIRENE kinetic transport code (www.eirene.de): gyro averaged ion kinetic up to edge-core interface



Here: C, C⁺, C²⁺, ... atomic carbon neutrals and ions

MAST: Geometry and exp. plasma data provided by S. Lisgo, UKAEA

Collisionality \rightarrow plasma fluid approximation multi-ion fluid (α ion species, $T_{\alpha} = T_{i}$, and electrons) multi-species Boltzmann eq. for neutrals (n neutral species) Braginskii, Reviews of Plasma Physics, 1965

Continuity equation for ions and electrons

$$\frac{\partial}{\partial t}n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i\right) = S_{n_i}$$

Momentum balance for ions and electrons



$$\begin{aligned} \frac{\partial}{\partial t} \left(m_i n_i \vec{V}_i \right) + \vec{\nabla} \cdot \left(m_i n_i \vec{V}_i \vec{V}_i \right) &= -\vec{\nabla} p_i - \vec{\nabla} \cdot \vec{\Pi}_i + Z_i e n_i \left(\vec{E} + \vec{V}_i \times \vec{B} \right) + \vec{R}_i + \vec{S}_{m_i \vec{V}_i} \\ -\vec{\nabla} p_e - e n_e \left(\vec{E} + \vec{V}_e \times \vec{B} \right) + \vec{R}_e &= 0 \end{aligned}$$

Energy balances for ions and electrons

$$\frac{\partial}{\partial t} \left(\frac{3}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) + \vec{\nabla} \cdot \left[\left(\frac{5}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) \vec{V}_i + \vec{\Pi}_i \cdot \vec{V}_i + \vec{q}_i \right] = \left(e n_i Z_i \vec{E} - \vec{R} \right) \cdot \vec{V}_i - Q_{ei} + S_E^i$$

$$\frac{\partial}{\partial t} \left(\frac{3}{2}n_e T_e\right) + \vec{\nabla} \cdot \left(\frac{5}{2}n_e T_e \vec{V}_e + \vec{q}_e\right) = -en_e \vec{E} \cdot \vec{V}_e + \vec{R} \cdot \vec{V}_i + Q_{ei} + S_E^e$$

ASIDE

Momentum balance for ions and electrons (Navier Stokes "Braginskii" equations)

$$\frac{\partial}{\partial t} \left(m_i n_i \vec{V}_i \right) + \vec{\nabla} \cdot \left(m_i n_i \vec{V}_i \vec{V}_i \right) = -\vec{\nabla} p_i - \vec{\nabla} \cdot \vec{\Pi}_i + Z_i e n_i \left(\vec{E} + \vec{V}_i \times \vec{B} \right) + \vec{R}_i + \vec{S}_{m_i \vec{V}_i}$$

In edge codes often used only for $v_{\alpha_{_{\rm II}}}$ the flow parallel to B-field

The cross field momentum balance is replaced by diffusion-convection ansatz:

$$v_{\alpha \perp} = -\frac{D_n^{\alpha}}{h_{\perp}} \partial_{\perp} \left(\ln n_{\alpha} \right) - \frac{D_p^{\alpha}}{h_{\perp}} \partial_{\perp} \left(\ln p_{\alpha} \right) + V_{\perp}$$

with ad hoc (anomalous?) $D_{\perp}, V_{\perp} \kappa_{\perp}, \eta_{\perp},$

e.g. Strahl code,.....

Fusion devices

TEXTOR (R=1.75 m), Jülich, GER ITER (R=6.2 m), Cadarache, FRA



JET (R=2.96 m), Oxford, UK



joint: EU



joint: world-wide

Fusion devices: typical transport code runtime

TEXTOR (R=1.75 m), Jülich, GER ITER (R=6.2 m), Cadarache, FRA



Why become transport codes so slow for ITER sized machines? (for same model, same equations, same grid size)

Because of more important plasma chemistry (increased non-linearity, non-locality, in sources).

Fluid equations for charged particles

Continuity equation for ions and electrons

$$\frac{\partial}{\partial t}n_i + \vec{\nabla} \cdot \left(n_i \vec{V}_i\right) = S_n$$

Momentum balance for ions and electrons

$$\frac{\partial}{\partial t} (m_i n_i \vec{V}_i) + \vec{\nabla} \cdot (m_i n_i \vec{V}_i \vec{V}_i) = -\vec{\nabla} p_i - \vec{\nabla} \cdot \vec{\Pi}_i + Z_i e n_i (\vec{E} + \vec{V}_i \times \vec{B}) + \vec{R}_i + \vec{S}_{m_i \vec{V}_i}$$
$$-\vec{\nabla} p_e - e n_e (\vec{E} + \vec{V}_e \times \vec{B}) + \vec{R}_e = 0$$

Energy balances for ions and electrons

$$\frac{\partial}{\partial t} \left(\frac{3}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) + \vec{\nabla} \cdot \left[\left(\frac{5}{2} n_i T_i + \frac{m_i n_i}{2} \vec{V}_i^2 \right) \vec{V}_i + \vec{\Pi}_i \cdot \vec{V}_i + \vec{q}_i \right] = \left(e n_i Z_i \vec{E} - \vec{R} \right) \cdot \vec{V}_i - Q_{ei} + \vec{S}_E^i \\ \frac{\partial}{\partial t} \left(\frac{3}{2} n_e T_e \right) + \vec{\nabla} \cdot \left(\frac{5}{2} n_e T_e \vec{V}_e + \vec{q}_e \right) = -e n_e \vec{E} \cdot \vec{V}_e + \vec{R} \cdot \vec{V}_i + Q_{ei} + \vec{S}_E^e$$

System of PDGL's with locally increasing dominating sources: "diffusion-reaction-equations" rather than pure CFD

Separating time scales in plasma chemistry:

Kinetic (transport) equation, one for each species $\frac{\partial f(E,\vec{\Omega})}{\partial t} + \frac{\partial f(E,\vec{\Omega})}{\partial t} + \frac{f}{\tau} = S(E,\vec{\Omega}) - v\sigma_a(E)f(E,\vec{\Omega})$

System then becomes analogous to:

$$\frac{\partial f}{\partial t} = \vec{M}\vec{f} + \vec{S}$$

for those f_i, for which the transport has been removed from kinetic equation

Separating time scales in plasma chemistry:

Kinetic (transport) equation, one for each species $\frac{\partial f(E,\vec{\Omega})}{\partial t} + v\vec{\Omega} \cdot \nabla f(E,\vec{\Omega}) + Forces = S(E,\vec{\Omega}) - v\sigma_a(E)f(E,\vec{\Omega})$ Transport

External source Absorption

$$+ \int_{0}^{\infty} dE' \int_{4\pi} d\vec{\Omega}' \Big[v' \sigma_s \Big(E' \to E, \vec{\Omega}' \cdot \vec{\Omega} \Big) f \Big(E', \vec{\Omega}' \Big) - v \sigma_s \Big(E \to E', \vec{\Omega} \cdot \vec{\Omega}' \Big) f \Big(E, \vec{\Omega} \Big) \Big]$$

Collisions

$$\frac{\partial \vec{f}}{\partial t} = \vec{M}\vec{f} + \vec{S}$$

for those f_i, for which the transport has been removed from kinetic equation

CR Models in Transport Codes ("bundled states")

- 1) System of N kinetic (or fluid) equations (PDGL, IGL)
- 2) select M species, remove transport term and explicit time derivative (Interpretation: their lifetime is short compared to transport time)
- 3) System reduced to N M transport equations plus one linear algebraic system (CR Model), of order M

The M states are in quasi steady state with the N – M transported species. CR models are QSS models (this is also known as "bundled state model")

Characteristics (=Trajectories) of kinetic transport equation here: MAST, UKAEA Culham, UK



EXAMPLE

Collision-radiative model (CR) [K. Sawada, T. Fujimoto, 1995] for H,p,H₂,H₂⁺ (and H*, H₂*, H₂^{+*} as fast QSS-species)

$$\frac{dn}{dt} = 0 = \sum_{q < p} C_{qp} n_e n_q - \sum_{q > p} C_{pq} n_e n_p - \sum_{q < p} F_{pq} n_e n_p - \sum_{q < p} A_{pq} n_p - \sum_{q < p} A_{pq} n_p + C_{1p} n_e n_1 + \frac{R_p n_e n_+}{P_2 p_e} + \frac{D_{H_2} n_e n_+}{P_2 p_e}$$

Similar for nH_2^* , nH_2^{+*} , total: ~ 100 species, N – M = 4

- C: electronic excitation; F: electronic de-excitation;
- A: radiative decay;
- **R**: recombination; S: ionization; D: dissociation.

How to select M "fast" states

 H_2 : are $H_2(v)$ "metastable" or QSS species In C_xH_v brake-up: which are QSS?

A sound mathematical procedure (from combustion and flame science): The Intrinsic Low Dimension Manifold (ILDM) technique. (but: very cumbersome to implement in transport codes) Based on spectral analysis of reaction system.

See :

Dauwe, Tytgadt, Reiter: "Automatic reduction of the hydrocarbon reaction Mechanisms in fusion edge plasmas, JUEL-4299, Nov. 2006, ISSN 0944-2952 and: <u>www.eirene.de/recent</u>reports

Example: MAST (UK)



Consistent Plasma-Gas-Radiation fields in MAST edge



Plasma flow (experiment + OSM Modelling) Gas flow (atomic and molecular) EIRENE

Courtesy: S.Lisgo et al., MAST Team, EPS 2007



Spectroscopy \rightarrow OSM transport modelling \rightarrow CR plasma chemistry modelling \rightarrow \rightarrow Quantitative comparison \rightarrow experimental validation of tokamak edge chemistry

Courtesy: S.Lisgo et al., MAST Team, EPS 2007

Transport-Simulations for ITER



Numerical tool for the edge plasma science: B2-EIRENE code package (FZJ-ITER)

Reiter, D., et al., Fusion Science and Technology 47 (2005) 172.



ITER, B2-EIRENE simulation, fully detached, T_e field



ITER, B2-EIRENE simulation, detached, n_e field



ITER, B2-EIRENE simulation, detached, n_A field



ITER, B2-EIRENE simulation, detached, n_{H2} field



Consequences for ITER design (B2-EIRENE): shift towards higher divertor gas pressure to maintain a given peak heat flux (Kotov et al., CPP, July 2006)

ITER divertor engineering parameter: target heat flux vs. divertor gas pressure



P_{PFR}: average neutral pressure in Private Flux Region

— 1996

(ITER physics basis1999)

 2003, neutral - neutral collisions

-+ molecular kinetics
 (D₂(v)+D⁺, MAR)

- 2005, + photon opacity



ITER design review 2007-2008: "Dome" re-design now considered ITER Divertor design is based upon "detachment"

Detachment is a chemically complex plasma state: "unknown territory" in fusion,

but well known in low temperature plasma physics

- gas-plasma friction,
- recombining plasmas,
- plasma cooling (radiation)

Current hypothesis: in the "detached state" is the divertor dynamics and chemistry is controlled by "Collisionality" (inv. Knudsen number)



Shot: 990429019, at 950ms, $<n_e>=1.5 \ 10^{20}$, $I_P=0.8 \ MA$, $B_{tor}=5.4 \ T$ OSM reconstruction (Lisgo et al., 2004)





D_γ (from D, D₂, D⁺,D₂⁺): **Profile matched**, but high by factor 2 Calibration? Atomic Data? Plasma reconstruction?

Results very sensitive eg. to T_e profile

H₂ molecule, status in present divertor code

More complete models available, still need to be integrated

compiled 2005





Neutral Plenum Pressure

Exp: 25 mTorr Calc 2D (2000) 3 mTorr Calc 2D (2003) 27 mTorr (better A&M data, better Plasma data, better codes)



Very good match: code - experiment But: Is there further edge physics that we are sure must be operative?

Additional leakage pathways:

 $2D \rightarrow 3D$ (see later)



3D Neutral Gas, A&M and PSI Modelling



3D divertor structures (toroidal gap and gussets, bypass and poloidal gap)

→strong toroidal variations in the divertor neutral pressure

Ionization by electron impact on neutral gas



Radiation transfer: opacity of Ly-lines

(though completely elementary, has long remained unnoticed in edge modelling) $h_V+H(1)\rightarrow H^*$, $H^*+e \rightarrow H+ 2e$ (additional path for ionization in dense, low T_e divertors)





Model validation in the presence of many free parameters:

include ALL edge physics that we are sure must be operative even while our capability to confirm these directly remains limited

Radiation transfer module: verification and validation using HID lamps



High Intensity Discharge Lamps



D2-36 W Automotive Material:Quartz

CDM-75 W Shop-Lighting Material:PCA



$2D \rightarrow 3D$

- Extending edge models towards predictive quality is a theoretical and experimental task
- Going from 2D CFD to 3D CFD is a computational physics task

- 0 3D recycling, reaction-diffusion problems: in hand
- 1: smooth particle hydrodynamics+ random walks (ITER, W7X, LHD)
- 2 Edge ergodization (TEXTOR-DED, DIIID: C-Coils, ELM-mitigation)

Tore Supra

Interior view of Tore Supra



Full toroidal limiter CIEL

dépôt de flux LPT avec TOKAFLU/OMBRAGE



Large Helical Device (LHD), Toki, Japan





Prediction: high source upstream, high flow speed, low T near target

TEXTOR-DED: smooth particle hydrodynamics Monte Carlo for non convective terms interpolated cell mapping for stochasticity



Typical runtime for a 3D edge modelling job (TEXTOR-DED case, single transport equation)



Conclusions/Outlook

Similar to previous steps: progress to ITER is based mainly on experimental and empirical extrapolation

guided by theory and aided by modelling

Present goal:

include all of edge physics that we are sure must be operative (opacity, A&M physics, surface processes, drifts..., even while our capability do confirm these directly remains limited.

Present upgrading:

- low temperature plasma chemistry
- consistent wall models
- drifts and electrical currents in the edge
- 2D →3D
- coupling to first principle edge turbulence codes
- code integration: Core- ETB edge (ELM modelling)

Summary: Edge Theory and Modelling

Where are we? A reality check

Compare with aircraft aerodynamics

Things in Common:

•Both use fluid models/codes as primary analysis tool

 In both cases one can get fairly far with 2D (ITER design) but in the end: 3D is needed

•Both involve a powerful controlling fluid-solid interaction/interface

•Both involve turbulence in an important way

•Both are applied sciences: What, Why, How (how can we make this application work?)

Summary: Edge Theory and Modelling

Where are we? A reality check

Compare with aircraft aerodynamics

The differences:

Aero: involves 2 states of matter. The Edge: minimum 3, sometimes all 4
Aero: involves no B or E fields, no currents, Maxw. Eq. play no role.

Edge: Maxwells eqs. as important as fluid eqs.

•Sub-sonic aero: largely incompressible flow. Our fluid is compressible

•Aero: one fluid. We: many fluids (electrons, ions, impurities...)

•Aero: no exchange of matter. For us: the exchanges are dominating

•Aero: some unsteady effects, but no equivalent to our powerful effects: ELMs...

•Aero: 2D flow field can be studied in small, cheep, wind tunnels,

done 1000's of times over 100 years

We need 2D (3D) fluid field for all fluids, around the entire edge (when? cost?)

Summary: Edge Theory and Modelling

Where are we? A reality check

Computational aircraft aerodynamics is still an active field of research.

Edge plasma: orders of magnitude more complex, orders of magnitude less R&D

If computational edge plasma science would be "largely in hand", it would be a miracle.

A major computational edge plasma science effort is needed, in order to avoid major code failures in the ITER design and operation

The JET divertor design philosophy

Michael Pick has used to describe the design of the JET divertor:

"The only way to do research is to tell the complete truth. And the truth is that research is often based partially on intuition, which is a perfectly acceptable basis for research in the face of a lack of evidence and verified predictive models.

We built the divertor based on what we thought would be a reasonable solution, based on simple extrapolation, models and intuition, leaving open the possiblities to change."

Still true for ITER, despite significant progress in edge plasma science and in predictive quality of models

 One and a half decade ago we lacked a credible solution to the divertor problem.

 With the discovery of the cold, detached, radiating divertor in the 1990s, we now have (the makings of) a divertor solution for high power magnetic confinement devices.

We now have enough understanding of "WHAT" (JET, Tore-Supra, D-IIID, ASDEX, LHD, W7AS,.....) to proceed with the "HOW" (to build ITER,...) Very little on the "WHY" question still, see lecture III But we are ready to go: Bring on ITER!





Compare to similar situation after first flight of Wright brothers The End

Reserve slides

Motivation – understanding SOL flows

Simplified – flow components in poloidal plane only



The Impurity Transport Code ERO

IV.) Applications of ERO

The ERO webpage – still under development ...

