

RAPTOR tutorial

code version 2.0

November 2017

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Outline

- **Part I - This talk**
 - Introduction to RAPTOR
 - Equations, physics model and numerical method
 - RAPTOR code structure: directories, data objects, functions
 - Version management - SVN
 - Where to get help
 - License agreement
- **Part II - Try it for yourself**
 - Work through the RAPTOR tutorials to familiarize yourself with options
 - Optionally try your own simulations

Basics of RAPTOR

- **RApid Plasma Transport simulatOR**
 - Fast transport code time evolution of 1D tokamak plasma profiles, designed for *real-time* and *control-oriented* use.
- **Solve coupled nonlinear PDEs for poloidal flux and T_e**
 - Assume fixed MHD equilibrium, parametrized actuators and transport
- **Numerics**
 - using cubic splines
 - implicit numerical solver.
 - Returns Jacobians w.r.t. state and inputs, and local linearization.
- **Modular**
 - Feedback controllers can be used for any actuator.
 - Easy to add more physics or more functionality.
- **Language/versioning**
 - Matlab (Simulink for real-time C code generation)
 - SVN for code version control

Equations solved by RAPTOR (1/2)

- **1D, (flux surface averaged) diffusion of poloidal flux**

$$\sigma_{\parallel} \left(\frac{\partial \psi}{\partial t} \Big|_{\hat{\rho}} - \frac{\hat{\rho} \dot{\Phi}_b}{2\Phi_b} \frac{\partial \psi}{\partial \hat{\rho}} \right) = \frac{F^2}{16\pi^2 \mu_0 \Phi_b^2 \hat{\rho}} \frac{\partial}{\partial \hat{\rho}} \left[\frac{g_2 g_3}{\hat{\rho}} \frac{\partial \psi}{\partial \hat{\rho}} \right] - \frac{B_0}{2\Phi_b \hat{\rho}} V'_{\hat{\rho}} j_{ni}$$

- Neoclassical conductivity, bootstrap current.
- Current drive sources as sums of gaussians or manual profiles,
- Boundary condition through total I_p or ψ_{edge} ,
- **Flux surface averaged temperature diffusion**

$$\frac{3}{2} (V'_{\hat{\rho}})^{-5/3} \left(\frac{\partial}{\partial t} \Big|_{\hat{\rho}} - \frac{\dot{\Phi}_b}{2\Phi_b} \frac{\partial}{\partial \hat{\rho}} \right) [(V'_{\hat{\rho}})^{5/3} n_e T_e] + \frac{1}{V'_{\hat{\rho}}} \frac{\partial}{\partial \hat{\rho}} \left(-\frac{g_1}{V'_{\hat{\rho}}} n_e \chi_e \frac{\partial T_e}{\partial \hat{\rho}} + \frac{5}{2} T_e \Gamma_e g_0 \right) = P_e$$

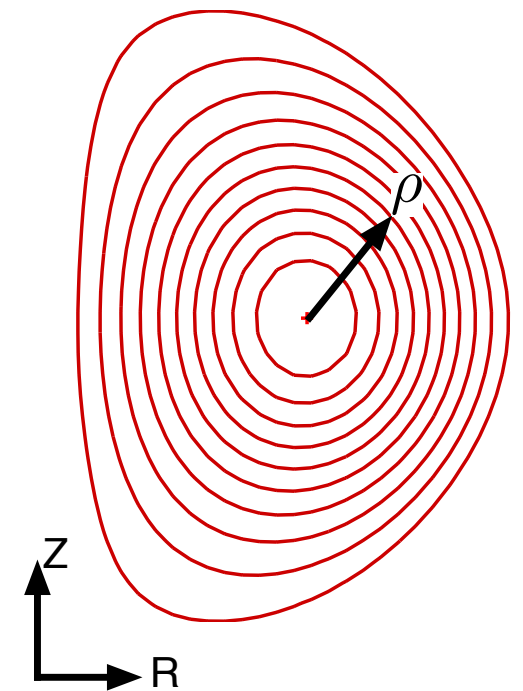
- Solve T_e and optionally T_i equation.
- Heat sources as sums of gaussians or manually prescribed
- Simple analytical sink models, + alpha power
- Ad-hoc model for thermal diffusivity with various transport models.
 - BgB [Erba 1998], Simple analytical [Felici PPCF 2012], qIkANN [Citrin NF 2015], Critical-gradient model [Teplukhina PPCF2017]

Equations solved by RAPTOR (2/2)

- **Flux surface averaged particle diffusion**

$$\frac{1}{V'_{\hat{\rho}}} \left(\frac{\partial}{\partial t} \Big|_{\hat{\rho}} - \frac{\dot{\Phi}_b}{2\Phi_b} \frac{\partial}{\partial \hat{\rho}} \hat{\rho} \right) [(V'_{\hat{\rho}}) n_s] + \frac{1}{V'_{\hat{\rho}}} \frac{\partial}{\partial \hat{\rho}} \left(-\frac{g_1}{V'_{\hat{\rho}}} D_s \frac{\partial n_s}{\partial \hat{\rho}} + g_0 V_s n_s \right) = S_s$$

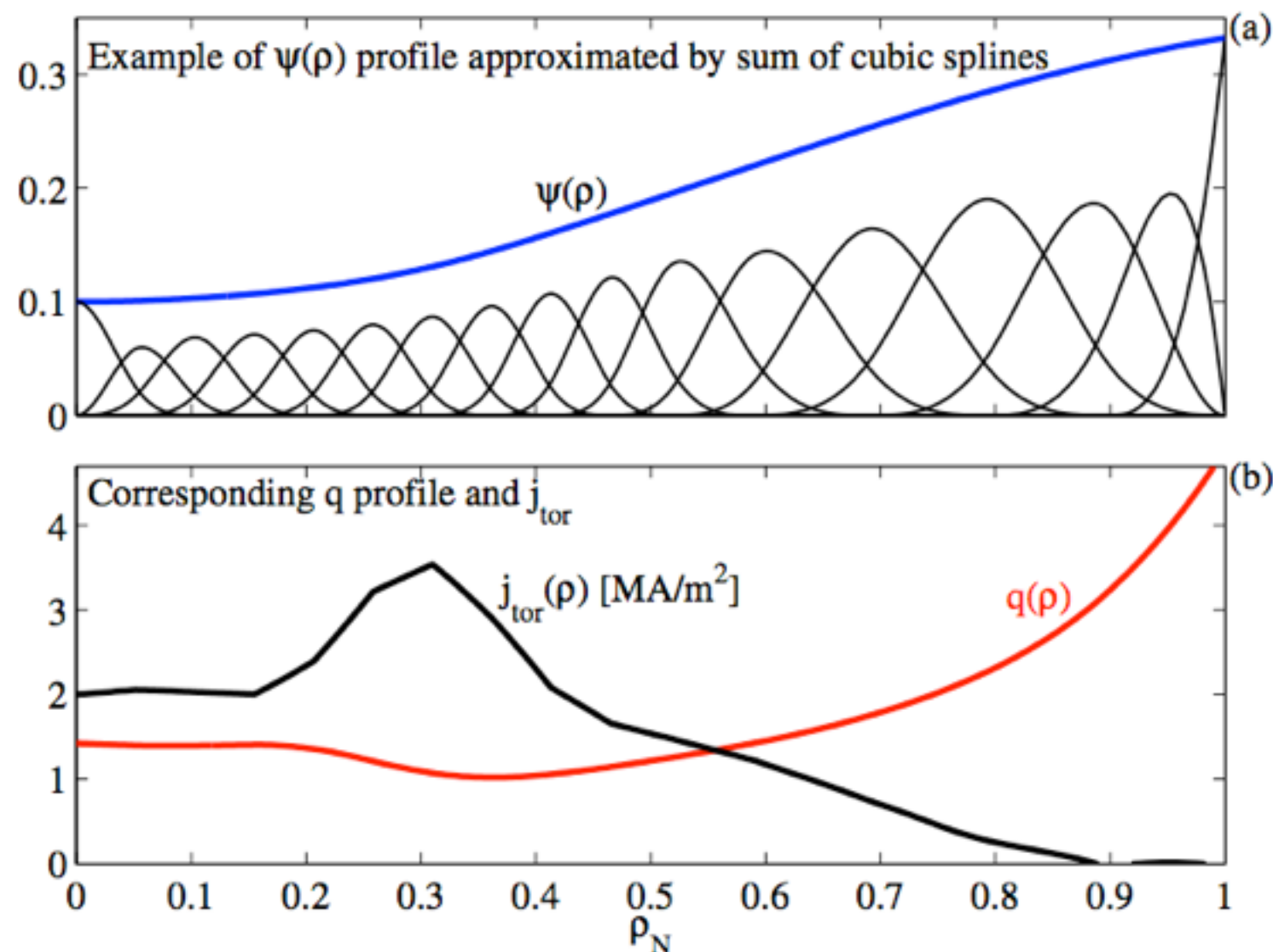
- For choice of species, electrons, ions, up to 3 impurities
- Non-simulated species can be set as fractions of other species, directly prescribed, or constrained by Z_{eff} and quasineutrality.
- **Magnetic equilibrium terms ($V', g_0, g_1, g_2, g_3, \Phi_{b..}$) taken from user-supplied equilibrium.**
 - GS equilibrium not evolved self-consistently
- **Other physics (optional)**
 - H-mode pedestal
 - MHD: Sawteeth and NTM



Some background: spatial discretization of profiles

- Express profile as sum of basis functions

$$\psi(\rho, t) = \sum_{\alpha=1}^{n_{sp}} \Lambda_{\alpha}(\rho) \hat{\psi}_{\alpha}(t) \quad \text{and} \quad T_e(\rho, t) = \sum_{\alpha=1}^{n_{sp}} \Lambda_{\alpha}(\rho) \hat{T}_{e\alpha}(t)$$



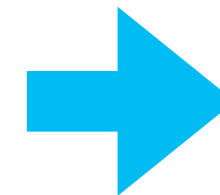
From Continuous time PDE to Discrete-time matrix ODE

- PDE with basis functions

$$\sum_{\alpha=1}^{n_{sp}} m \frac{d\hat{y}_{\alpha}(t)}{dt} \Lambda_{\alpha}(\rho) = \sum_{\alpha=1}^{n_{sp}} \hat{y}_{\alpha}(t) \frac{\partial}{\partial \rho} \left[g \frac{\partial \Lambda_{\alpha}(\rho)}{\partial \rho} \right] + k j,$$

- Multiply left and right by Λ_b and integrate

$$\sum_{\alpha=1}^{n_{sp}} \frac{d\hat{y}_{\alpha}(t)}{dt} \underbrace{\int_0^{\rho_e} m \Lambda_{\beta} \Lambda_{\alpha} d\rho}_{M_{\beta\alpha}(t)} = - \sum_{\alpha=1}^{n_{sp}} \hat{y}_{\alpha}(t) \underbrace{\left[\int_0^{\rho_e} g \frac{\partial \Lambda_{\beta}}{\partial \rho} \frac{\partial \Lambda_{\alpha}}{\partial \rho} d\rho \right]}_{=D_{\beta\alpha}} + \underbrace{\left[g \Lambda_{\beta} \frac{\partial y}{\partial \rho} \right]_0^{\rho_e}}_{=l_{\beta}} + \underbrace{\left[\int_0^{\rho_e} \Lambda_{\beta} k j d\rho \right]}_{=s_{\beta}}.$$



$$\mathbf{M} \frac{d\hat{\mathbf{y}}}{dt} = -\mathbf{D} \hat{\mathbf{y}} + \mathbf{l} + \mathbf{s},$$

NB: M,D,l,s depend nonlinearly on (y,u)

- Temporal discretization:

$$\dot{x}(t_k) = (x_{k+1} - x_k) / \Delta t, \quad x(t_k) = \theta x_{k+1} + (1 - \theta) x_k, \quad u(t_k) = u_k.$$

Implicit numerical scheme for time-evolution

- PDE(ρ, t) \rightarrow discretize \rightarrow Nonlinear ODE at each time step:

$$\tilde{f}(x_{k+1}, x_k, u_k) = \tilde{f}_k = 0 \quad \forall k$$

- At each time step, given state x_k , inputs u_k at time step k ,

- Take steps in Newton descent direction d

$$\mathcal{J}_{k+1}^k d = \tilde{f}_k,$$

- Need Jacobian, obtained from analytical expression for all the derivatives (copious application of chain rule)

$$\mathcal{J}_{k+1}^k = \frac{\partial \tilde{f}_k}{\partial x_{k+1}}$$

- Iterate until residual $f_k < \text{tolerance}$
- Go to next time step
- Store Jacobians at each time step

Parameter sensitivity of profile evolution

- Time evolution depends on mode parameters
 - One example: a transport model parameter
 - Another example: a parameter defining the input trajectory

$$\tilde{f}(x_{k+1}, x_k, u_k) = \tilde{f}_k = 0 \quad \forall k$$

- Differentiating with respect to parameter p , we get the *sensitivity equation*

$$0 = \frac{d\tilde{f}_k}{dp} = \frac{\partial \tilde{f}_k}{\partial x_{k+1}} \frac{\partial x_{k+1}}{\partial p} + \frac{\partial \tilde{f}_k}{\partial x_k} \frac{\partial x_k}{\partial p} + \frac{\partial \tilde{f}_k}{\partial u_k} \frac{\partial u_k}{\partial p} + \frac{\partial \tilde{f}_k}{\partial p}$$

- Linear ODE for dx_k/dp , solve while evolving nonlinear PDE: *Forward sensitivity analysis*
- Jacobians df_k/dx_k , df_k/dx_{k+1} are known from Newton iterations
- Computational cost proportional to p
- dx_k/dp gives the linearization of the state trajectories in the parameter space

$$T_e(\rho, t)|_{p=p_0+\delta p} \approx T_e(\rho, t)_{p_0} + \frac{\partial T_e}{\partial x} \frac{\partial x}{\partial p} \delta p$$

Equilibrium definition

- Presently, RAPTOR uses profile information from a CHEASE run (2D fixed-boundary GS solver)
 - $V'(\rho)$, $g_{0,1,2,3}(\rho)$ etc
- Pre-calculated equilibria exist for TCV, AUG, JET, ITER
 - May scale them with R_0 , B_0 as necessary
- Analytical equilibria could be added.
- For other equilibria, will need to run CHEASE
 - talk to F. Felici or O. Sauter
- 2-way coupling to general 2D equilibria (from fast GS solver or parametrized profiles) envisioned.

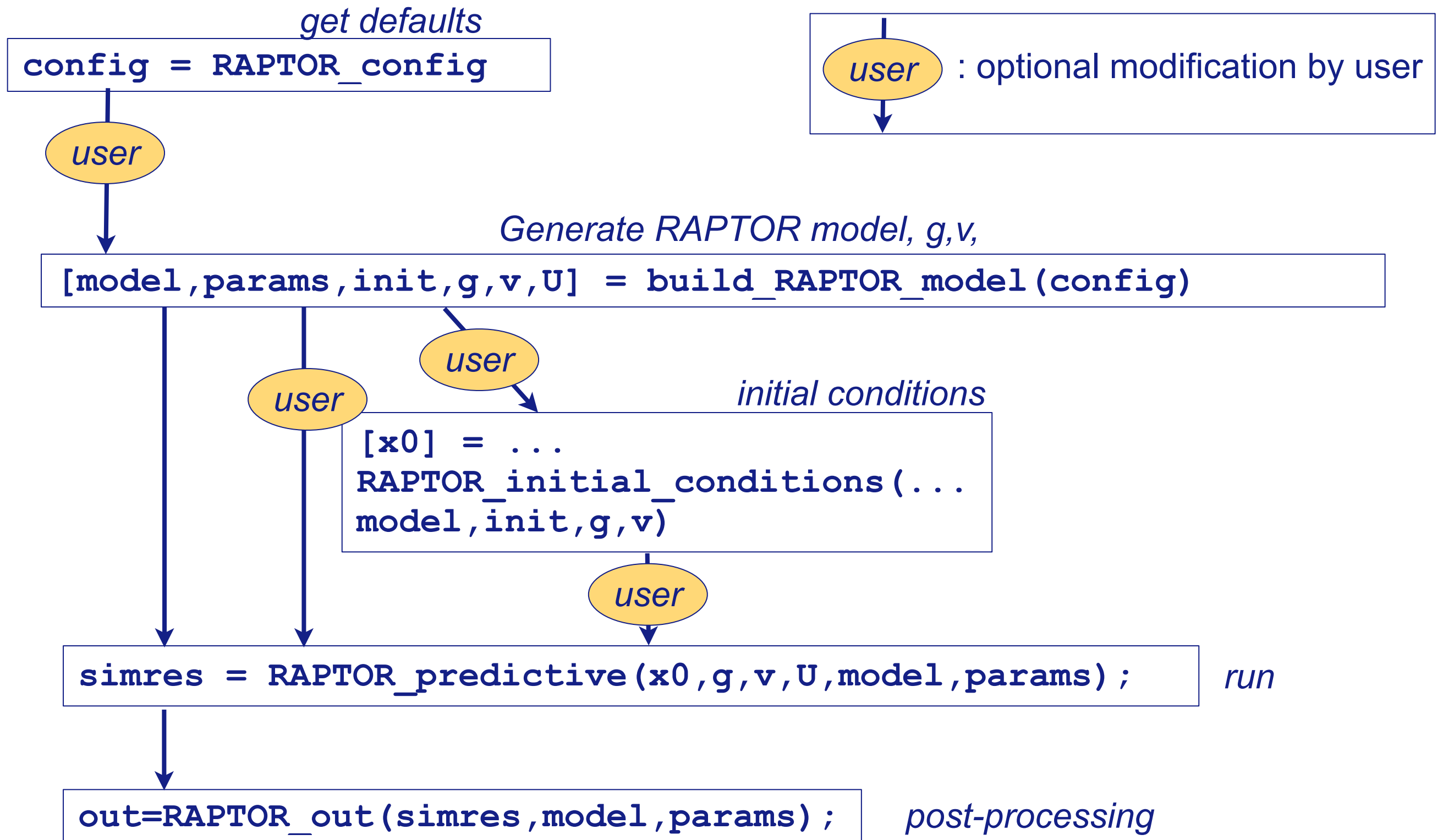
RAPTOR data objects: structures

- **config**: contains configuration info for generating RAPTOR model and parameter structures
 - Physics (transport coefficients, heating¤t drive, boundary conditions, ...)
 - Numerics (radial and temporal grid, spline order, solver tolerances, ...)
 - Environment (paths etc), run-time plot and display options
- **model**: contains all pre-calculated data (matrices etc) that should not be changed manually.
 - Spline basis matrices, radial grid, boundary condition type, transport model type
 - Fixed profiles/quantities which do not change in time.
- **params**: contains all parameters that can be tuned between runs.
 - Time grid
 - Parameters for transport models, other physics modules
 - Numerics / debugging flags
- **init**: parameters for generating initial conditions

RAPTOR data objects: time-varying vectors

- **x**: state quantities which the code solves for.
- **v**: pre-known but time-varying kinetic profile quantities.
- **g**: geometry-related quantities
- **u**: Actuator inputs
- **In terms of these objects, a time step in the code solves**
 - $\mathbf{x}_{k+1} = \mathbf{f}(\mathbf{x}_k, \mathbf{g}_k, \mathbf{v}_k, \mathbf{u}_k, \text{model}, \text{params})$

RAPTOR workflow



Directory structure

- **RAPTOR/**
 - **code:** core code files.
 - **tests:** tests to check that code runs correctly
 - **demos:** demonstration files and tutorials.
 - **doc:** documentation
 - **equils:** equilibrium files defining equilibrium profiles.
 - **projects:** projects that are built “on top of” RAPTOR
 - **optimization:** Tools for nonlinear optimization
 - **data:** store temporary data here (not versioned)
 - **personal:** store personal scripts here (not versioned)
 - **license:** license agreement
 - **RT:** Real-time implementations (Simulink)
 - **tokamakdensitymodel:** a related code for density evolution
 - [Blanken FusEngDes 2017]

Version control - SVN (Subversion)

- Hosted on SPCSVN at SPC-EPFL Lausanne (T.M. Tran)
- Code is developed in trunk, regular “tags” at stable releases
 - This presentation applies to tags/release-2.0
- Many tutorials exist for svn. Important commands (UNIX):
 - Check out the RAPTOR trunk from server to local directory
 - `svn co https://spcsvn.epfl.ch/repos/RAPTOR/tags/release-2.0 ./RAPTOR`
 - Check differences between local and current version
 - `svn stat -uv`
 - Revert to version on server (beware! undoes local changes!)
 - `svn revert my_file.m`
 - Commit local changes to server
 - `svn ci my_file.m -m“Comment”`
 - Get latest updates
 - `svn update`
- Contact F. Felici to get read/write access to SVN repository

Where to get help

- **Getting started: tutorials and demo files**
 - in the /demos directory, type 'help demos' and do the tutorials
 - Run some standard scenarios in /demos/standard_scenarios.
- **Explanations on the meaning various parameters:**
 - As comments next to default value definition.
 - RAPTOR_config (for general parameters)
 - Inside the module to which the parameter applies (for the rest)
- **Physics and numerics**
 - F. Felici thesis, online <http://dx.doi.org/10.5075/epfl-thesis-5203>
 - F. Felici NF 2011 <http://dx.doi.org/10.1088/0029-5515/51/8/083052>
 - F. Felici PPCF 2012 <http://stacks.iop.org/0741-3335/54/i=2/a=025002>
- **Equation details**
 - RAPTOR equation document in /doc directory
- **E-mail: f.felici@tue.nl**

User's license and conditions

The undersigned has received a copy of RAPTOR under the conditions that:

- 1.- The code does not change its name even if modified.
- 2.- Modifications of the code that are developed are made available to the CRPP.
- 3.- Results produced with the original or the modified versions of RAPTOR should appropriately reference the original publications:

For use of RAPTOR as a real-time interpretative code:

F. Felici et al. Nuclear Fusion **51**(8), p.083052 (2011)

For the predictive version of RAPTOR or its use in nonlinear optimization routines:

F. Felici et.al. Plasma Physics and Controlled Fusion **54**(2), p.025002 (2012)

- 4.- RAPTOR nor its progeny may be transferred or made available to other research groups without the written authorisation from the CRPP.