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CFD Analysis of Steam Turbines with the IAPWS Standard on the Spline-Based Table Look-up Method (SBTL) for the Fast Calculation of Real Fluid Properties

Project of the IAPWS Task Group "CFD Steam Property Formulation"

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"IAPWS Guideline on the Fast Calculation of Steam and Water Properties With the Spline-Based Table Look-Up Method (SBTL)"

Evaluation Committee:

Adam Novy, Doosan Skoda   Francisco Blangetti, Alstom Power   Reiner Pawellek, STEAG
Julien Bonifay, Siemens Energy   Ingo Weber, Siemens Energy

ASME Turbo Expo 2015, June 15 – 19, Montréal, Canada

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Contents:

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Fluid Property Calculations in CFD Analyses of Steam Turbines

Need for accurate fluid properties in CFD:

- Density deviations $\Delta\rho$ result in:
  - inaccurate mass flows and velocities (speeds and directions)
- Deviations in caloric properties, e.g. the isobaric heat capacity c_p, result in:
  - inaccurate energy and entropy balances

Deviations in calculated fluid properties lead to less accurate simulation results and less efficient steam turbines!

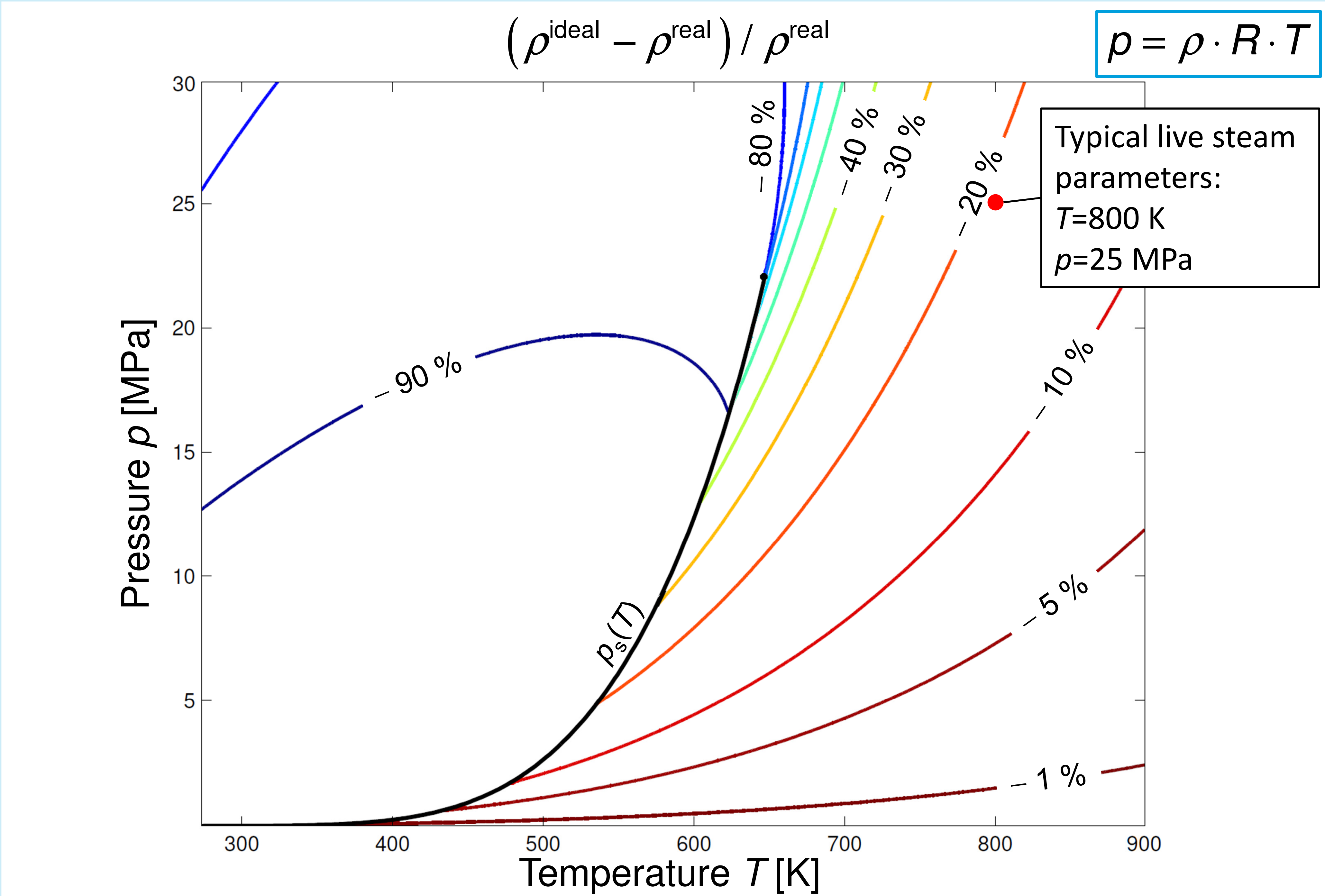
Available property calculation algorithms for water and steam:

- Ideal gas model
- Cubic equations of state (Peng-Robinson, Redlich-Kwong, …)
- Industrial standard IAPWS-IF97 (fundamental equations)
- Table look-up methods (such as the bi-linear interpolation in ANSYS CFX)

Requirements for property calculations in CFD:

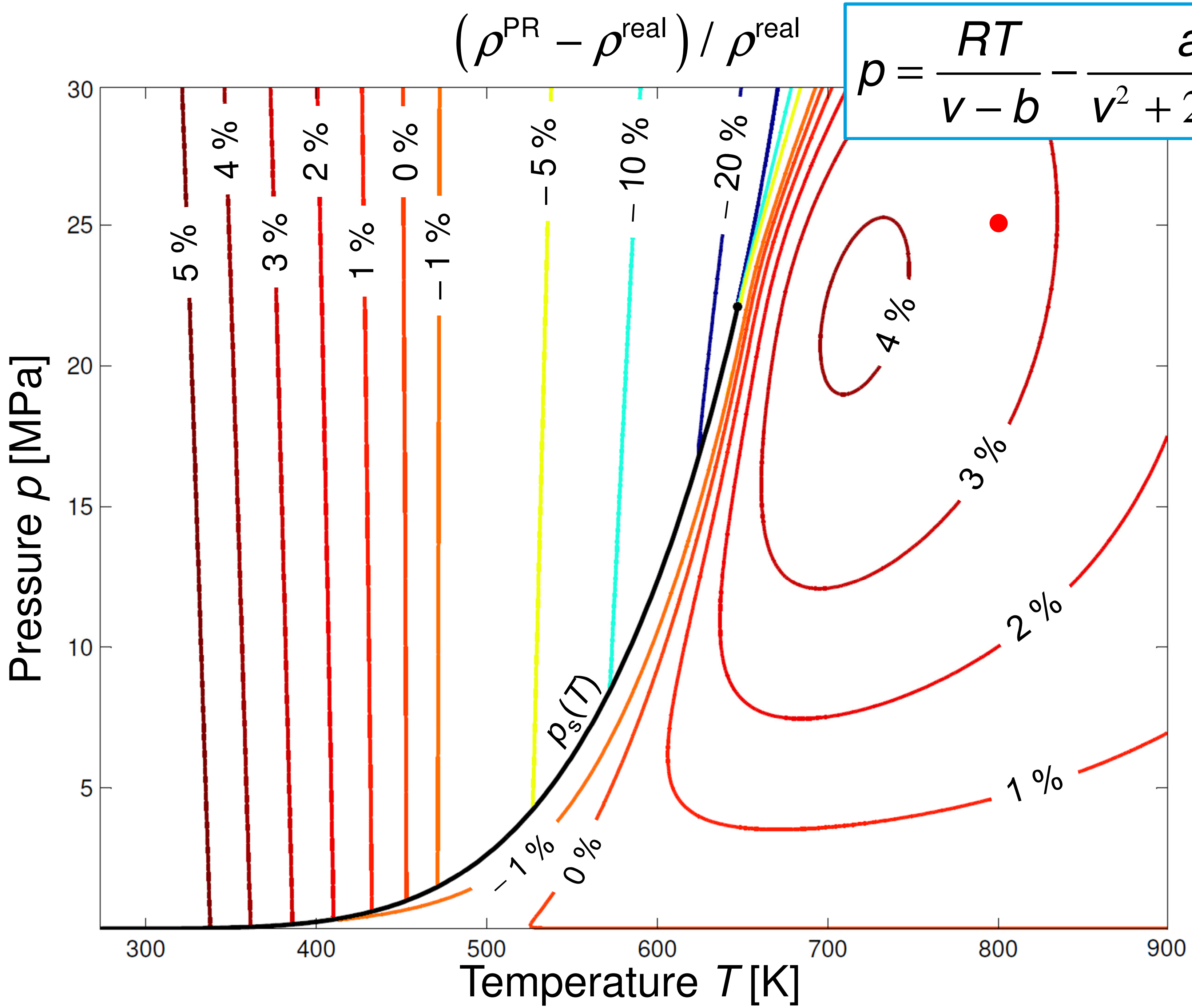
- Accuracy
- Computing speed

Deviations in density from real fluid (water and steam): ideal gas

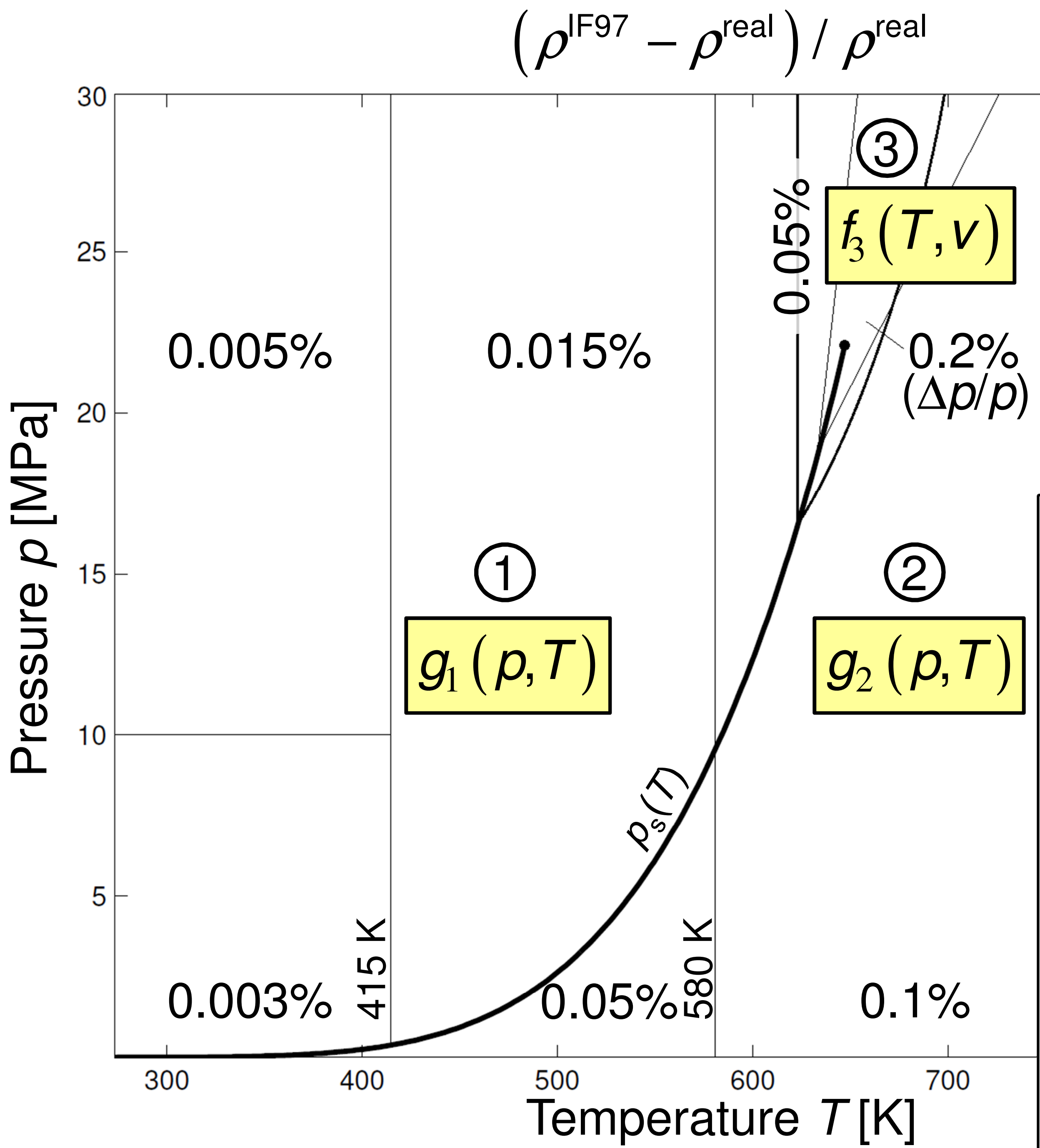


Deviations in density from real fluid (water and steam): cubic equation of state (Peng-Robinson)

$$p = \frac{RT}{v-b} - \frac{a(T)}{v^2 + 2bv - b^2}$$



Uncertainties in density of water and steam: IAPWS-IF97



Region 2:

$$\frac{g_2(p,T)}{R \cdot T} = \gamma^0(\pi,\tau) + \gamma^r(\pi,\tau)$$

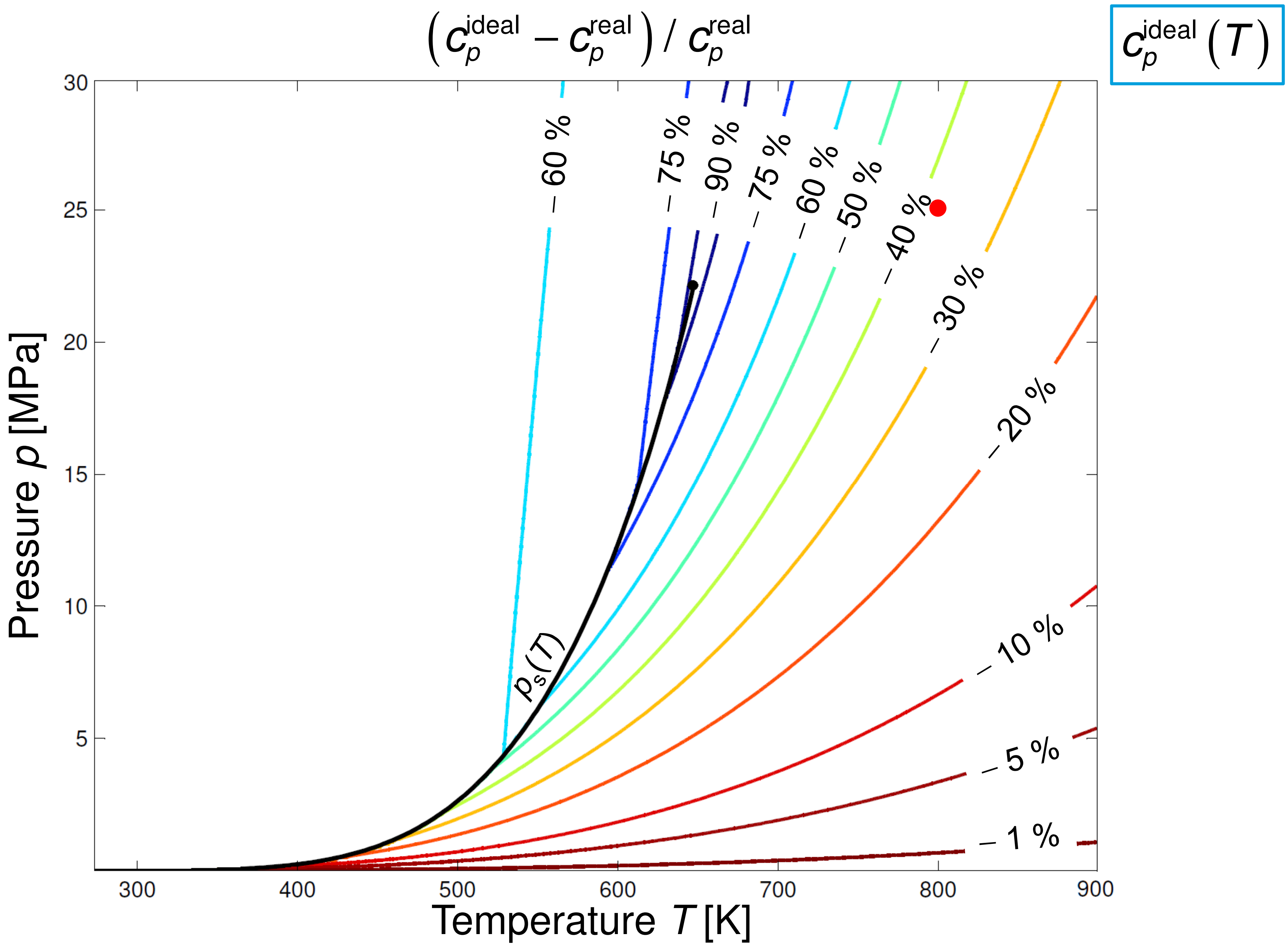
$$\tau = \frac{T^*}{T} \qquad \pi = \frac{p}{p^*}$$

$$\gamma^0(\pi,\tau) = \ln\pi + \sum_{i=1}^{9} n_i^0 \tau^{J_i^0}$$

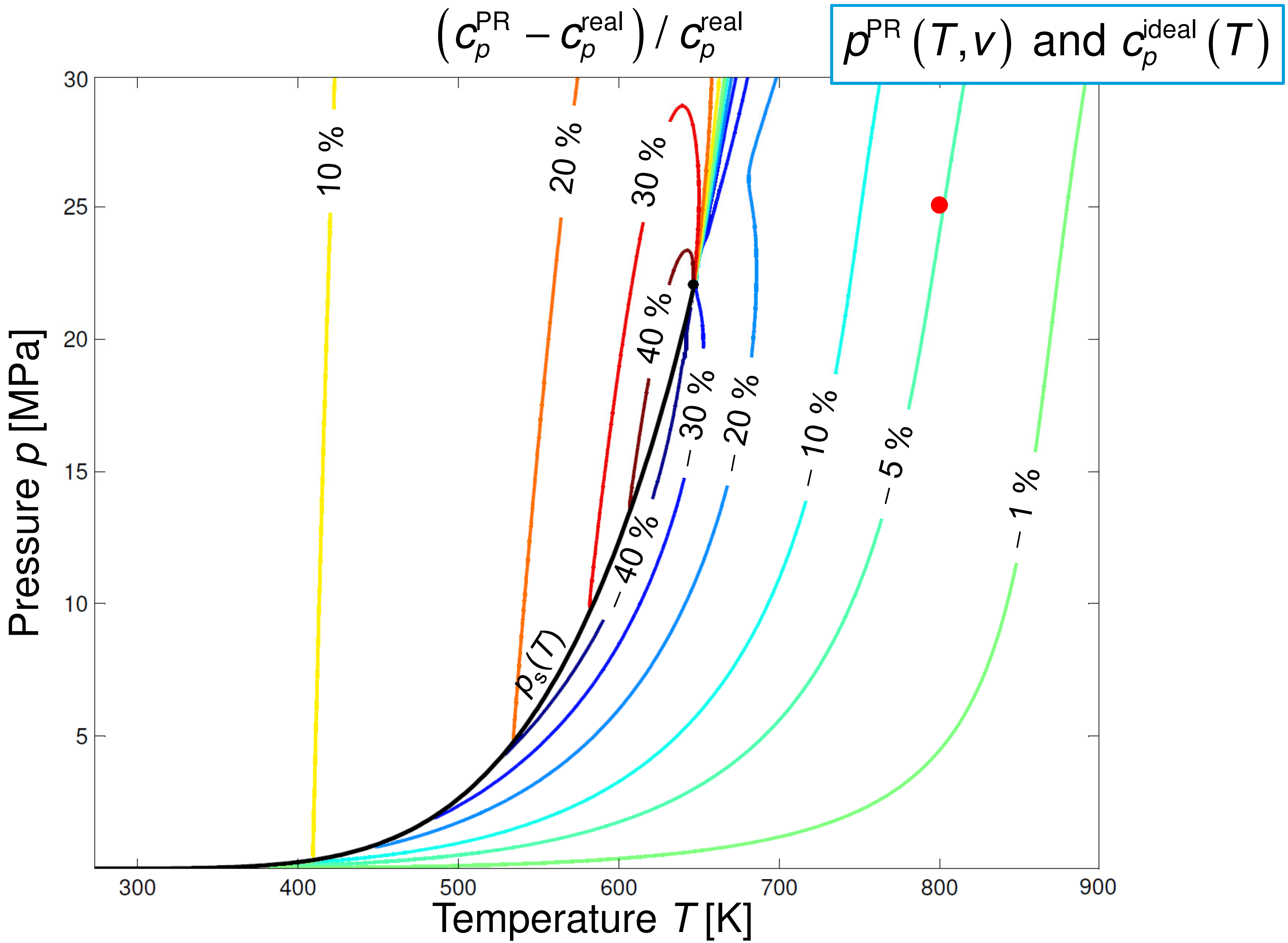
$$\gamma^r(\pi,\tau) = \ln\pi + \sum_{i=1}^{43} n_i \pi^{I_i} (\tau - 0.5)^{J_i}$$

$$v(\pi,\tau)\frac{p}{RT} = \pi(\gamma_\pi^0 + \gamma_\pi^r)$$

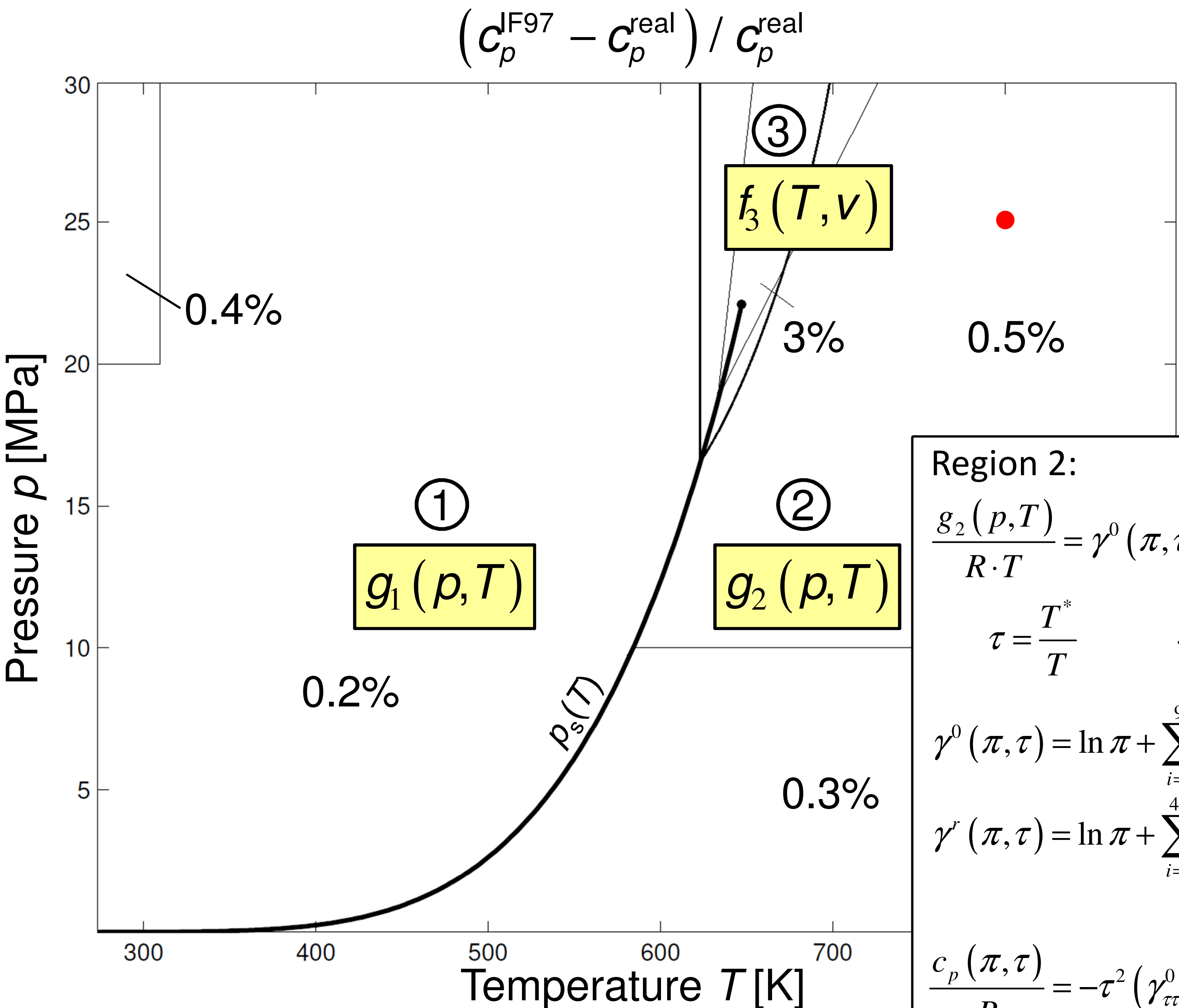
Deviations in isobaric heat capacity from real fluid (water and steam): ideal gas



Deviations in isobaric heat capacity from real fluid (water and steam): cubic equation of state + $c_p^{\text{ideal}}(T)$



Uncertainties in isobaric heat capacity of water and steam: IAPWS-IF97



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$$\gamma^r(\pi,\tau) = \ln\pi + \sum_{i=1}^{43} n_i \pi^{I_i} (\tau - 0.5)^{J_i}$$

$$\frac{c_p(\pi,\tau)}{R} = -\tau^2 \left(\gamma_{\tau\tau}^0 + \gamma_{\tau\tau}^r\right)$$

Fluid Property Calculations in CFD Analyses of Steam Turbines

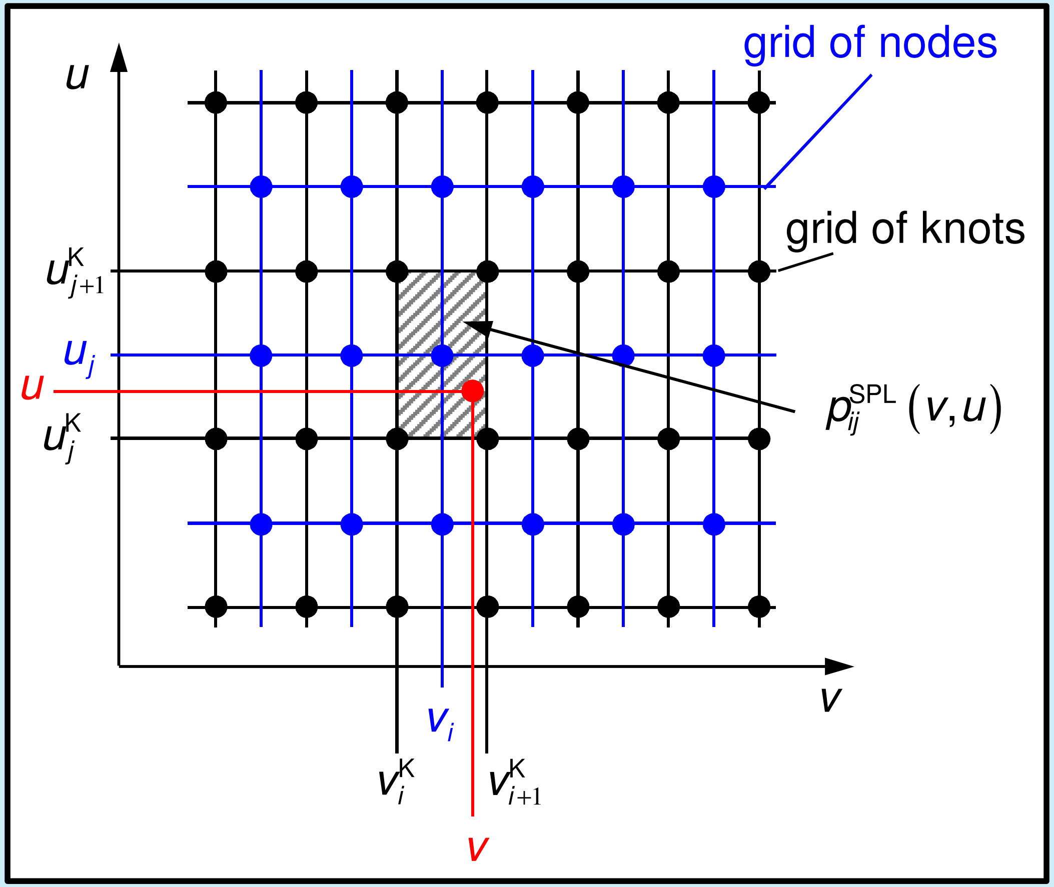
	Available property calculation algorithms for water and steam			
Requirements	**Ideal gas**	**Cubic equation of state**	**Ind. standard IAPWS-IF97**	**Table look-up methods**
Accuracy	$\lvert\Delta\rho\rvert \leq 20\ \%$ $\lvert\Delta c_p\rvert \leq 50\ \%$	$\lvert\Delta\rho\rvert \leq 4\ \%$ $\lvert\Delta c_p\rvert \leq 30\ \%$	$\lvert\Delta\rho\rvert \leq 0.3\ \%$ $\lvert\Delta c_p\rvert \leq 0.5\ \%$	depends on table size and algorithm
Computing speed	very high	acceptable	too slow	high

Application of a Spline-Based Table Look-Up Method to available equations of state (standards):

- Results of the underlying formulation can be reproduced with high accuracy and high computing speed
- Spline functions represent property functions continuously
- Forward and backward functions, e.g. $p(v,u)$ and $u(p,v)$, can be calculated with complete numerical consistency

Fundamentals of the Spline-Based Table Look-Up Method (SBTL)

Generation of a spline function $p^{SPL}(v,u)$ from an underlying eq. of state $p^{EOS}(v,u)$:



- **Generation of a rectangular grid of nodes:**
  - each node is calculated from the underlying equation of state:

$$p_{i,j}(v_i,u_j) = p^{EOS}(v_i,u_j)$$

- **Variable transformations of *v*, *u*, and *p*:**
  - enhance accuracy
  - transform the range of state
- **Cell definition in the grid of knots:**
  - spline-polynomial:

$$p_{ij}^{SPL}(v,u) = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ijkl}(v-v_i)^{k-1}(u-u_j)^{l-1}$$

  - intersects the inner node
  - continuous function and first derivatives
- **Optimization for:**
  - required accuracy
  - maximum computing speed
  - minimum amount of data (table size)
- **Providing the look-up table with the determined spline coefficients**

Property calculation within CFD:

- transform *v* und *u*
- cell (*i*,*j*) determination
- computation of the spline polynomial
- inverse transformation of *p*

Fundamentals of the Spline-Based Table Look-Up Method (SBTL)

Calculation of inverse spline functions (Example: bi-quadratic polynomial):

$$p_{ij}^{\mathrm{SPL}}(v,u) = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ijkl}\,(v - v_i)^{k-1}(u - u_j)^{l-1}$$

$$u_{ij}^{\mathrm{INV}}(p,v) = \frac{\left(-B \pm \sqrt{B^2 - 4AC}\right)}{2A} + u_j$$

where
$$A = a_{ij13} + \Delta v_i\left(a_{ij23} + a_{ij33}\Delta v_i\right)$$
$$B = a_{ij12} + \Delta v_i\left(a_{ij22} + a_{ij32}\Delta v_i\right)$$
$$C = a_{ij11} + \Delta v_i\left(a_{ij21} + a_{ij31}\Delta v_i\right) - p$$

and
$$\Delta v_i = (v - v_i)$$
$$(\pm) = \mathrm{sign}(B)$$

- **The inverse spline function is numerically consistent with its forward function.**
- **The inverse function can be calculated without any iteration.**

Spline Functions of (*v*,*u*) and Inverse Spline Functions Based on IAPWS-IF97

Calculation of inverse spline functions:

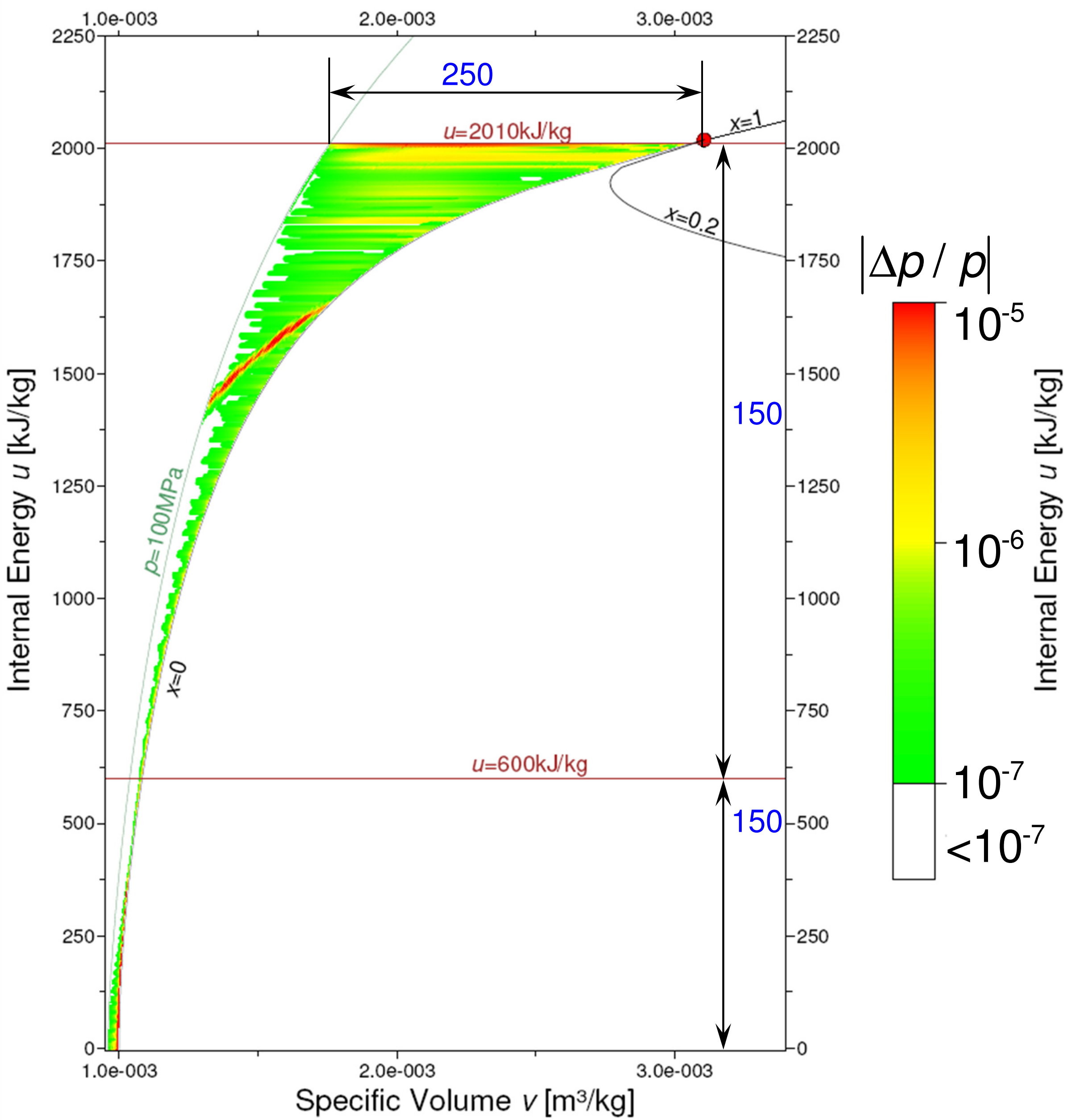
Spline functions of (*v*,*u*):

		(*p*,*v*):	(*u*,*s*):
Pressure	$p^{\mathrm{SPL}}(v,u)$ →	$u^{\mathrm{INV}}(p,v)$ → $T^{\mathrm{SPL}}, s^{\mathrm{SPL}}, w^{\mathrm{SPL}}, \eta^{\mathrm{SPL}}, \lambda^{\mathrm{SPL}}(v, u^{\mathrm{INV}})$	
Temperature	$T^{\mathrm{SPL}}(v,u)$		
Spec. entropy	$s^{\mathrm{SPL}}(v,u)$ →		$v^{\mathrm{INV}}(u,s)$ → $p^{\mathrm{SPL}}, T^{\mathrm{SPL}}, w^{\mathrm{SPL}}, \eta^{\mathrm{SPL}}, \lambda^{\mathrm{SPL}}(v^{\mathrm{INV}},u)$
Speed of sound	$w^{\mathrm{SPL}}(v,u)$		
Dynamic viscosity	$\eta^{\mathrm{SPL}}(v,u)$		
Therm. conductivity	$\lambda^{\mathrm{SPL}}(v,u)$		

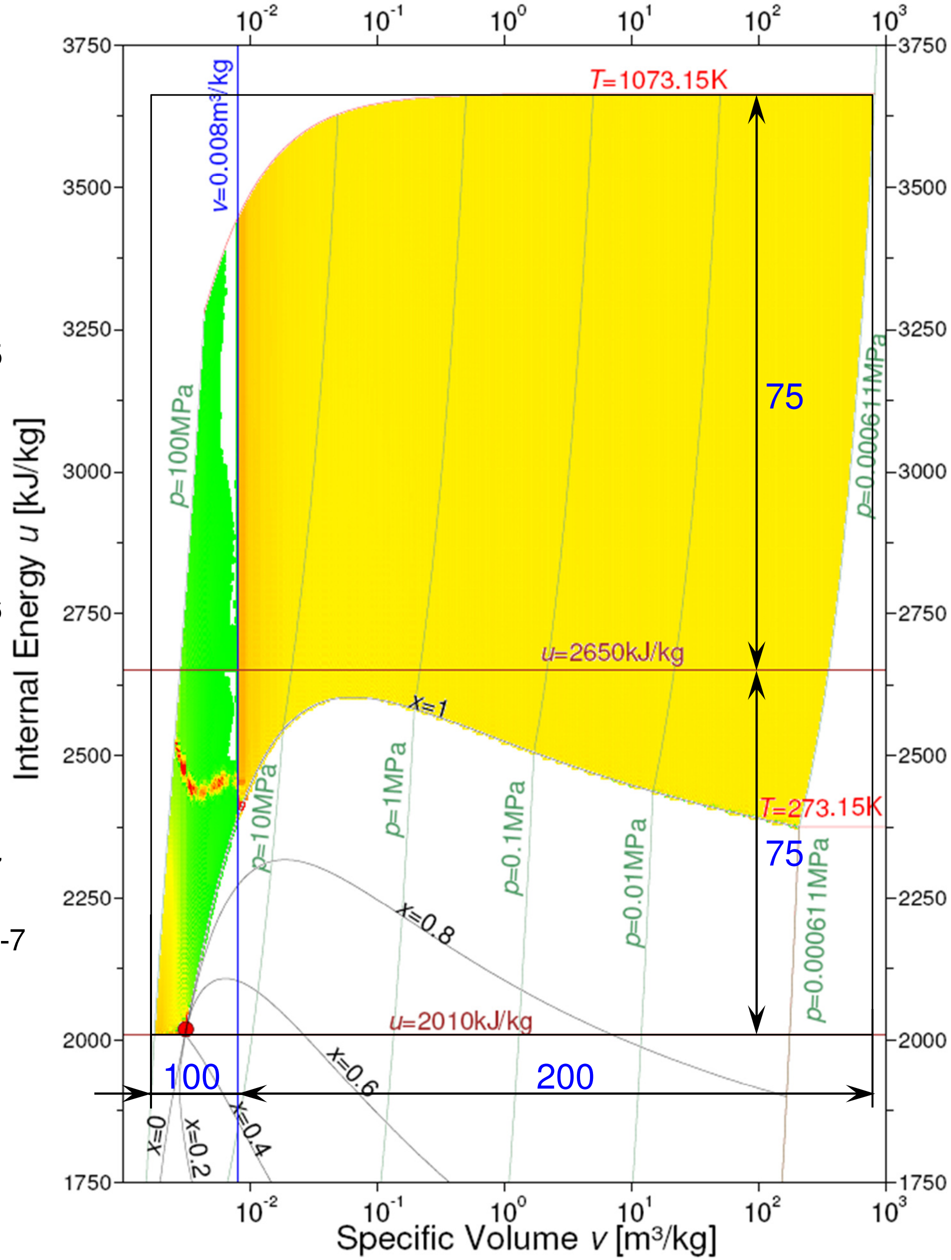
- **All thermodynamic and transport properties including derivatives and backward functions are calculated without iterations.**
- **Forward and backward functions are calculated with complete numerical consistency.**

Accuracy and Computational Speed of SBTL Functions for Water and Steam – Deviations from IAPWS-IF97

→ Spline function $p_L(v,u)$:



→ Spline function $p_G(v,u)$:



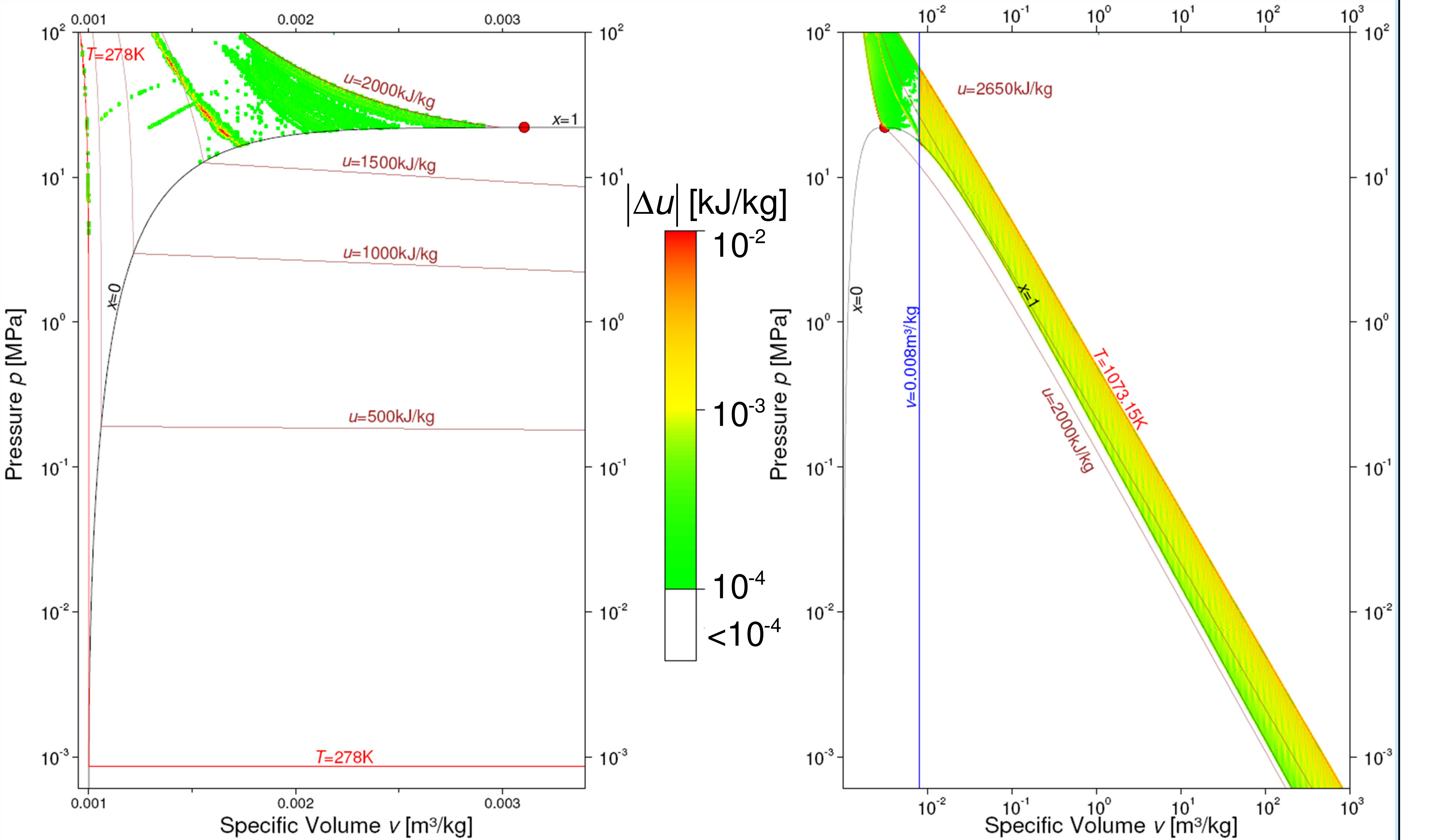
Transformations:

$\bar{v}$ scaled between $v(100\text{MPa}, u)$ and $v'(u)$

$\bar{v} = \ln(v)$

Accuracy and Computational Speed of SBTL Functions for Water and Steam – Deviations from IAPWS-IF97

→ **Inverse spline function $u_L(p,v)$:** → **Inverse spline function $u_G(p,v)$:**



➢ **Inverse spline functions are numerically consistent with their forward spline functions.**

Accuracy and Computational Speed of SBTL Functions for Water and Steam – Deviations from IAPWS-IF97

SBTL function		Max. deviation (L)	Max. deviation (G)
$p(v,u)$	$p \leq 2.5$ MPa	$\lvert \Delta p_L / p \rvert < 0.12\ \%$	$\lvert \Delta p_G / p \rvert < 0.001\ \%$
	$p > 2.5$ MPa	$\lvert \Delta p_L \rvert < 0.6\ \text{kPa}$	
$T(v,u)$		$\lvert \Delta T_L \rvert < 1\ \text{mK}$	$\lvert \Delta T_G \rvert < 1\ \text{mK}$
$s(v,u)$		$\lvert \Delta s_L \rvert < 10^{-6}\ \text{kJ kg}^{-1}\ \text{K}^{-1}$	$\lvert \Delta s_G \rvert < 10^{-6}\ \text{kJ kg}^{-1}\ \text{K}^{-1}$
$w(v,u)$		$\lvert \Delta w_L / w \rvert < 0.001\ \%$	$\lvert \Delta w_G / w \rvert < 0.001\ \%$
$\eta(v,u)$		$\lvert \Delta \eta_L / \eta \rvert < 0.001\ \%$	$\lvert \Delta \eta_G / \eta \rvert < 0.001\ \%$

⇩

- **Spline-based property functions reproduce the industrial standard IAPWS-IF97 with high accuracy (10 – 100 ppm).**

Accuracy and Computational Speed of SBTL Functions for Water and Steam – Computing time comparisons with IAPWS-IF97

Computing Time Ratio $CTR = \frac{\text{Computing time of the calculation from IAPWS-IF97}}{\text{Computing time of the calculation from the spline function}}$

	IAPWS-IF97 Region				
SBTL function	**1 (liquid)**	**2 (vapour)**	**3 (critical)**	**4 (two-phase)**	**5 (high-temp.)**
$p(v,u)$	130	271	161	19.6	470
$T(v,u)$	161	250	158	20.6	442
$s(v,u)$	164	261	160	17.8	449
$w(v,u)$	199	310	234	-	471
$\eta(v,u)$	197	309	239	-	-
$u(p,v)$	2.0	6.4	2.8	5.6	3.2
$v(u,s)$	43.5	66.4	78.8	16.2	134

Processor: Intel Xeon – 3,2GHz

Operating system: Windows7 (32 Bit)

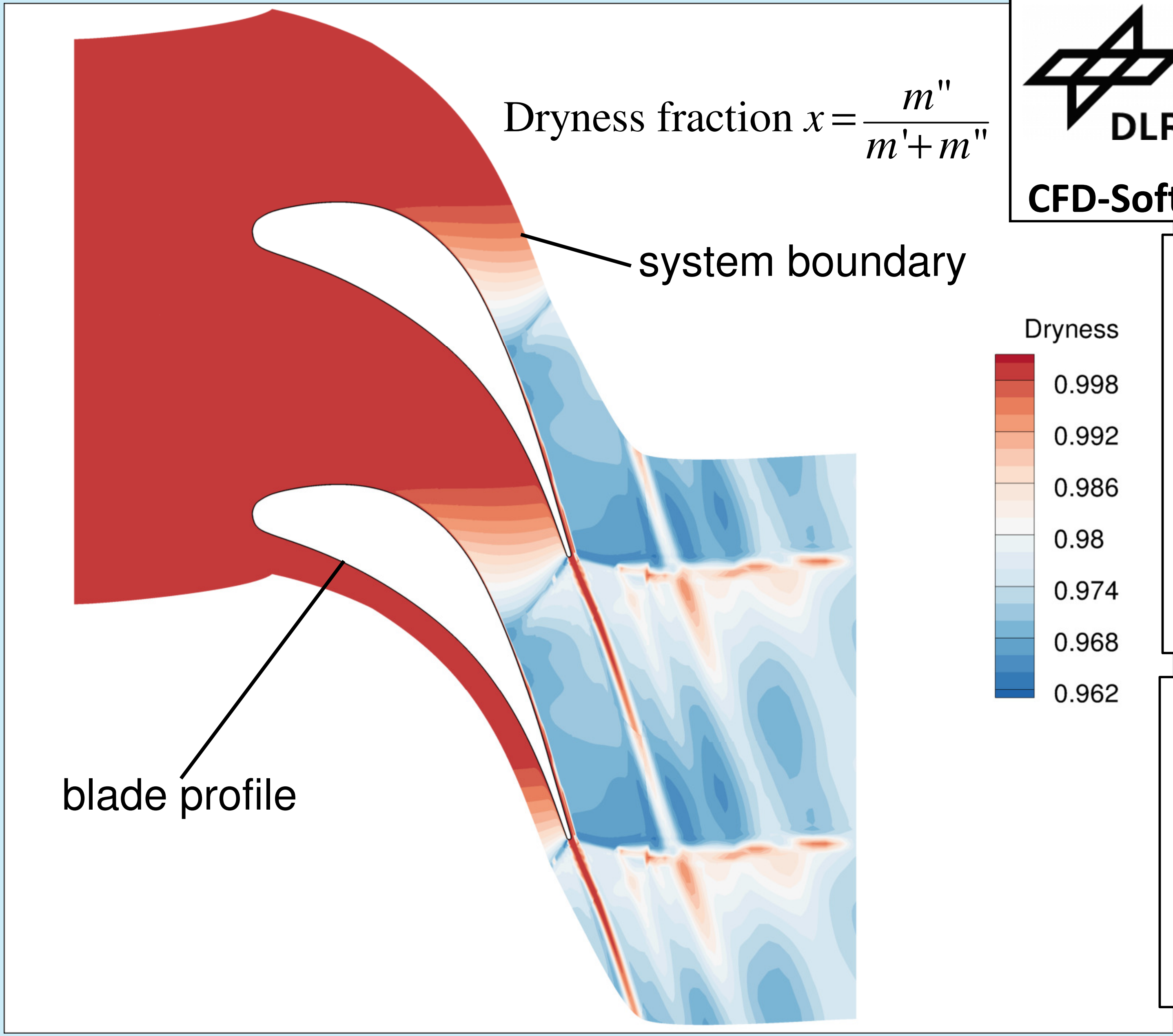
Compiler: Intel Composer XE 2011

➢ **Computing times are reduced by factors up to 300 (500)!**

Application of the SBTL Method in CFD – Condensing Steam Flow Around a Fixed Blade (White et al.)

Dryness fraction:

$$\text{Dryness fraction } x = \frac{m''}{m' + m''}$$



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CFD-Software TRACE (DLR)

Test-case L3:

Inlet conditions:

- Tot. press.: 41.7 kPa
- Tot. temp.: 357.5 K (ΔT_s=+7.5 K)

Outlet conditions:

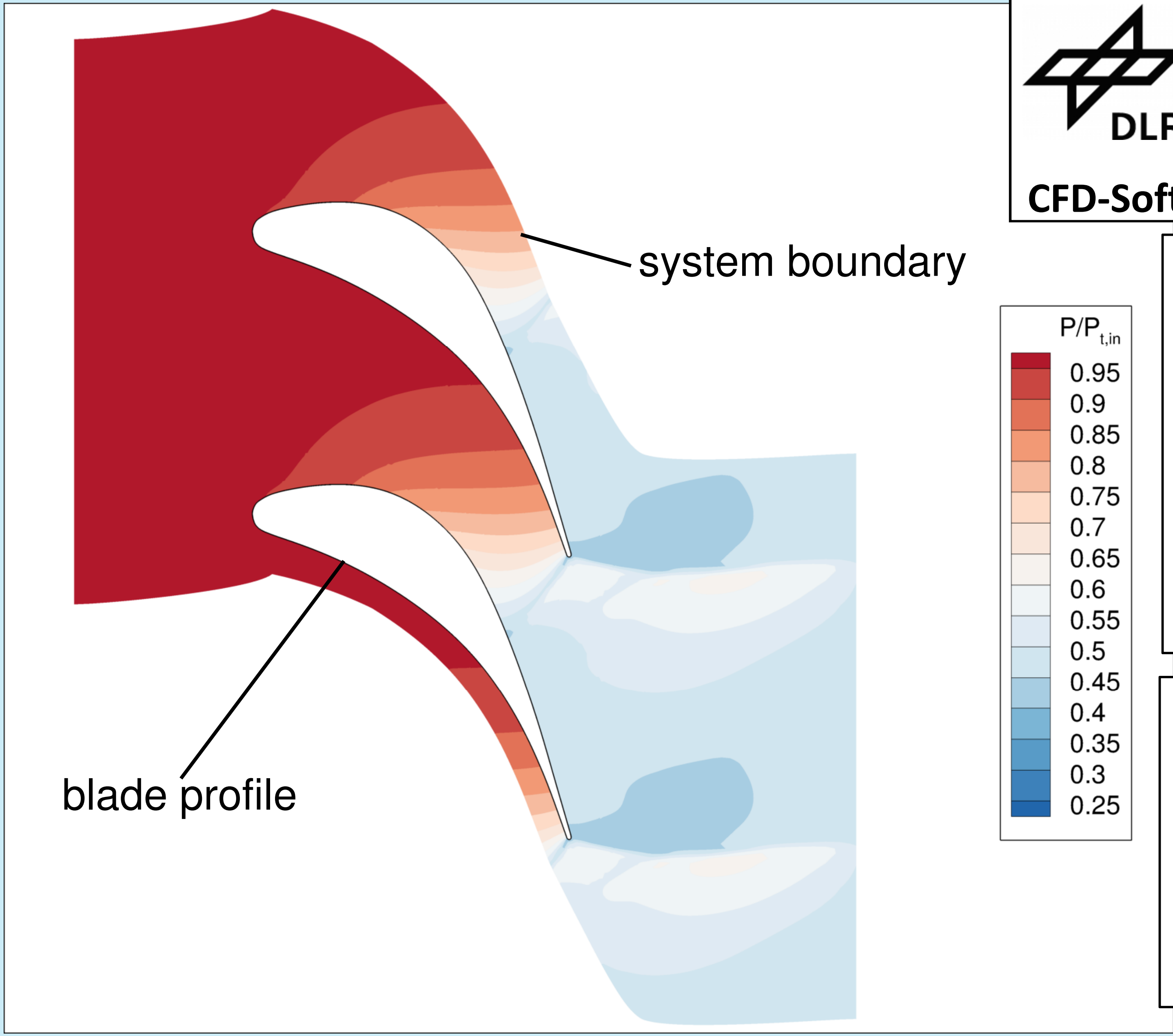
- Stat. pressure: 20.6 kPa

Assumptions:

- equilibrium condensation (no sub-cooling considered)
- homogeneous two-phase flow

Application of the SBTL Method in CFD – Condensing Steam Flow Around a Fixed Blade (White et al.)

Pressure distribution:



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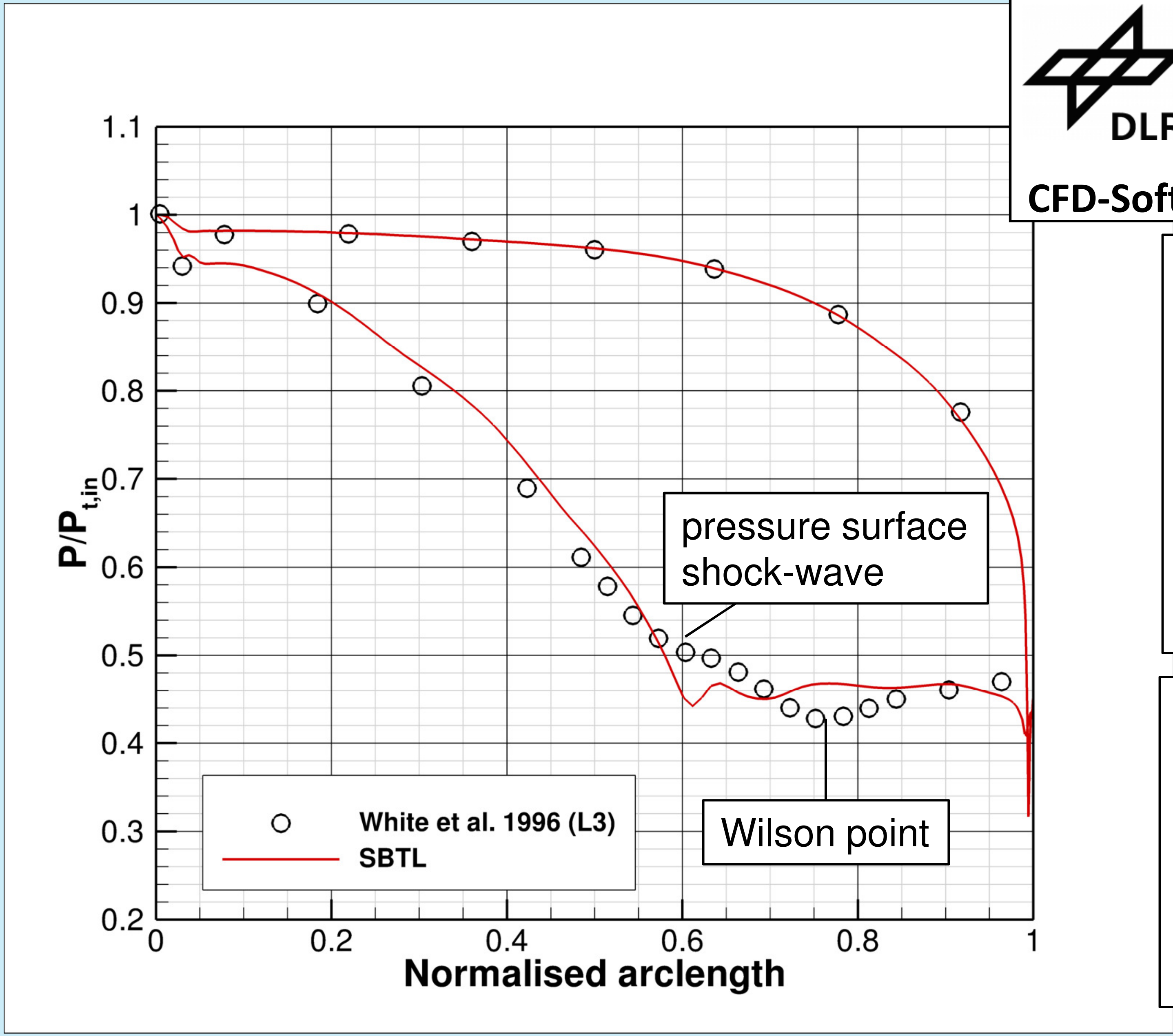
Application of the SBTL Method in CFD – Condensing Steam Flow Around a Fixed Blade (White et al.)

Pressure coefficient along the blade profile:



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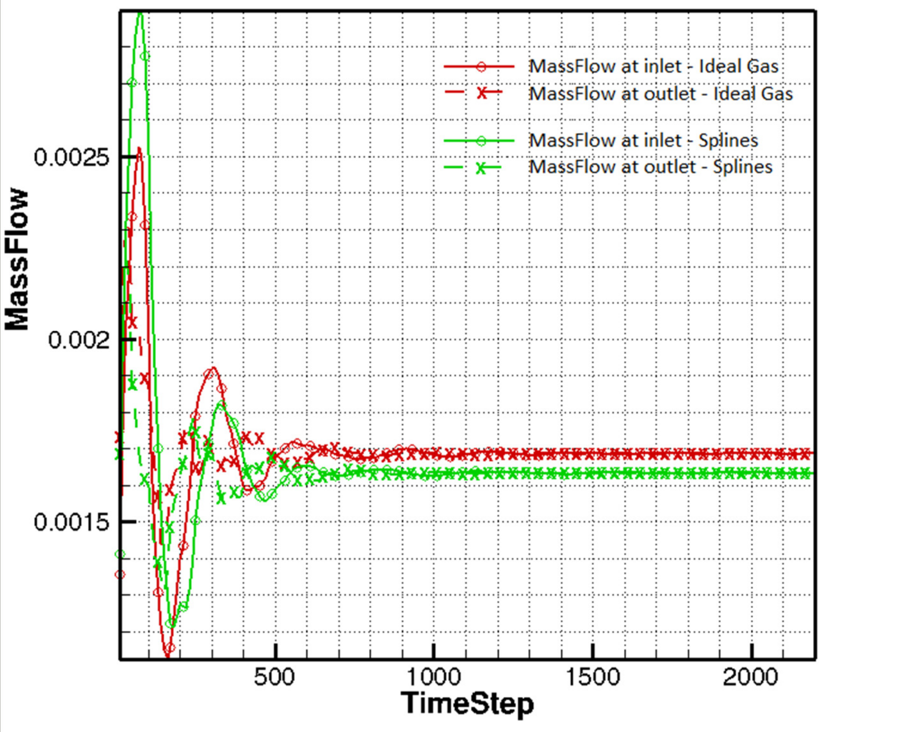
Application of the SBTL Method in CFD –
Condensing Steam Flow Around a Fixed Blade (White et al.)

Convergence:



CFL-Factor (Courant–Friedrichs–Lewy-Factor)=20

- **Calculation with SBTL functions:**
  - high speed of convergence because of complete numerical consistency
  - calculation accomplished after 1:50min/1000 steps

- **Comparison to calculation with ideal gas model:**
  - calculation accomplished after 1:20min/1000 steps

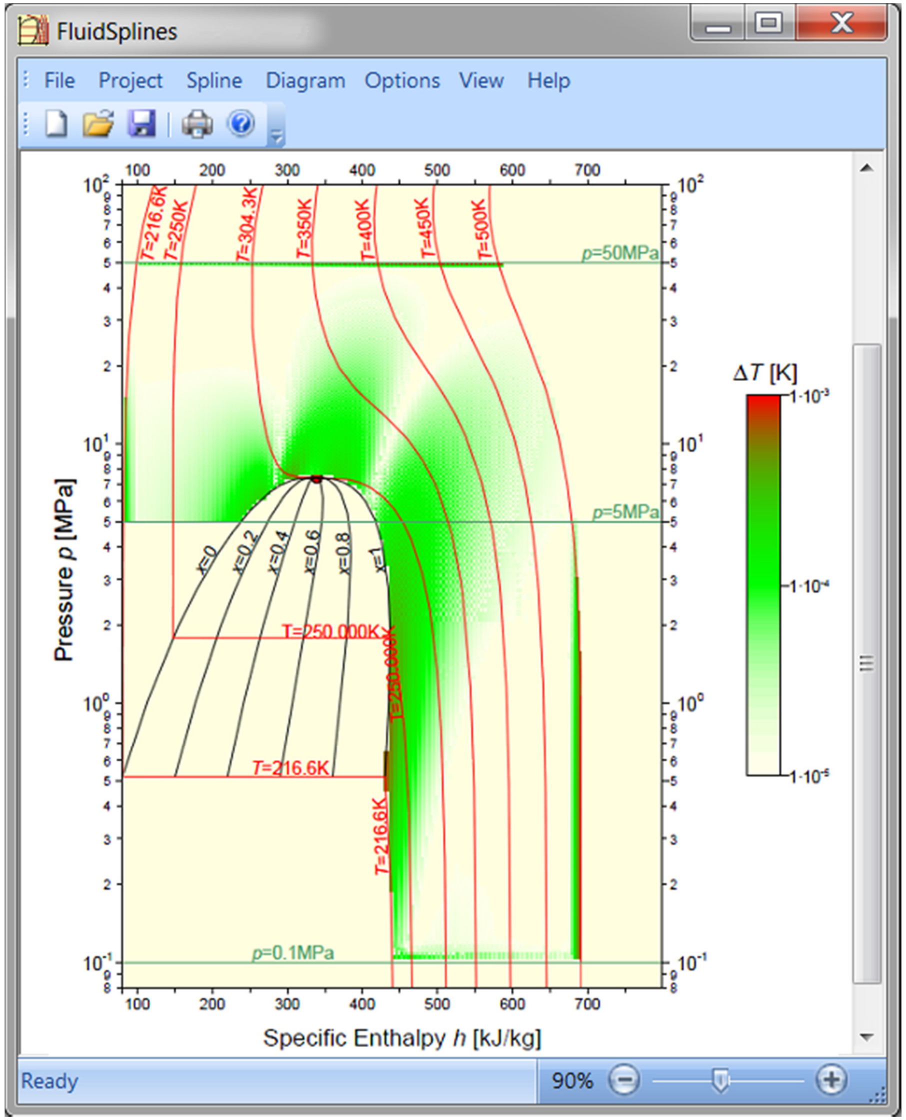
- **Calculation is approx. 6-10 times faster than the IAPWS-IF97 implementation in TRACE.**
- **Consideration of real fluid behavior with the SBTL Method requires only 40% additional computing time in comparison to a calculation with the ideal gas model.**
- **Practical calculations:**
  - **stage groups in 3D**
  - **non-stationary processes**

Computing time: several hours/days

Generation of SBTL Functions for Specific Demands

FluidSplines

Software for generating
spline-based property functions



Input:
(Thermodynamic Properties)

REFPROP©

Property-Libraries
(Zittau/Goerlitz Univ.)

Generation of SBTL-Functions for:
- specified range of validity
- required accuracy

Additional Features:
- generation of inverse spline-functions
- accuracy tests
- computing time tests

Output:
- optimized source code for high computing speed
- static/dynamic libraries
- documentation of accuracy and computing speed

Summary

- **Spline-Based Table Look-Up Method (SBTL):**
  - **Provides high accuracy and high computing speed at the same time**
  - **Property functions of available fundamental equations/standards are reproduced with an accuracy of 10 – 100 ppm - the results of a process simulation will not change**
  - **Computing speeds can be increased by factors > 100 in comparison to the calculation from fundamental equations**
  - **Complete numerical consistency of forward and backward functions is possible**
- **Applicability in Computational Fluid Dynamics (CFD) has been demonstrated**
  - **Enables consideration of the real fluid behavior with high accuracy**
  - **6-10 times faster than simulations with IAPWS-IF97**
  - **Only 40% slower than simulations with the ideal gas model**
  - **Next step: implementation of a nucleation model, heterogeneous two-phase flow**
- **SBTL functions for specific demands can be generated with FluidSplines:**
  - **Tailored for the required range of validity and accuracy**
  - **Applicable for any property function and any fluid**
- **Proposal:**

"IAPWS Guideline on the Fast Calculation of Steam and Water Properties With the Spline-Based Table Look-Up Method (SBTL)"

Thank you for your attention!