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# **A New IAPWS Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL)**

**Project of the IAPWS Task Group “CFD Steam Property Formulation”**

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# **A New IAPWS Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL)**

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- Requirements for Property Calculations in Extensive Process Simulations
- Fundamentals of the Spline-Based Table Look-Up Method (SBTL)
- SBTL Functions of:
  - $(v,u)$  and Inverse Functions of  $(p,v)$  and  $(u,s)$
  - $(p,h)$  and Inverse Functions of  $(p,T)$ ,  $(p,s)$ , and  $(h,s)$
- Application of the SBTL Method in CFD (TRACE, Developed at DLR)
- FluidSplines: SBTL Functions for Specific Demands
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# Requirements for Property Calculations in Extensive Process Simulations

## Computational Fluid Dynamics (CFD)

Flow analysis of power plant components



## Heat-Cycle Calculations (HCC)

Power plant design - process optimization



### Demands on Property Calculations

- Density deviations result in inaccurate mass flows and velocities
- Deviations in caloric properties result in inaccurate energy and entropy balances

Deviations lead to less accurate simulation results!

⇒ **Accurate property calculations are required.**

- Property functions are called millions of times

⇒ **Property functions need to be extremely fast.**

- CFD:
  - small volume elements
  - small time steps

- HCC of non-stationary processes, real-time process optimizations:
  - small time steps

⇒ **Inverse functions must be numerically consistent with their forward functions, e.g.  $u(p,v)$  and  $p(v,u)$ .**

# Available IAPWS-Formulations for Water and Steam

## Scientific Formulation IAPWS-95

Fundamental equation:  $\Phi = \frac{f}{R_m \cdot T} = \Phi^0(\tau, \delta) + \Phi^r(\tau, \delta) \quad \tau = \frac{T_c}{T} \quad \delta = \frac{\rho}{\rho_c}$

Ideal part:  $\Phi^0(\tau, \delta) = \ln(\delta) + n_1^0 + n_2^0 \cdot \tau + n_3^0 \cdot \ln(\tau) + \sum_{i=4}^8 n_i^0 \cdot \ln[1 - \exp(-\gamma_i^0 \cdot \tau)]$

Residual part:  $\Phi^r(\tau, \delta) = \sum_{i=1}^7 n_i \cdot \delta^{d_i} \cdot \tau^{t_i} + \sum_{i=8}^{51} n_i \cdot \delta^{d_i} \cdot \tau^{t_i} \cdot \exp(-\delta^{c_i}) +$   
 $+ \sum_{i=52}^{54} n_i \cdot \delta^{d_i} \cdot \tau^{t_i} \cdot \exp[-\alpha_i \cdot (\delta - \varepsilon_i)^2 - \beta_i \cdot (\tau - \gamma_i)^2] + \sum_{i=55}^{56} n_i \cdot \Delta^{b_i} \cdot \delta \cdot \psi$

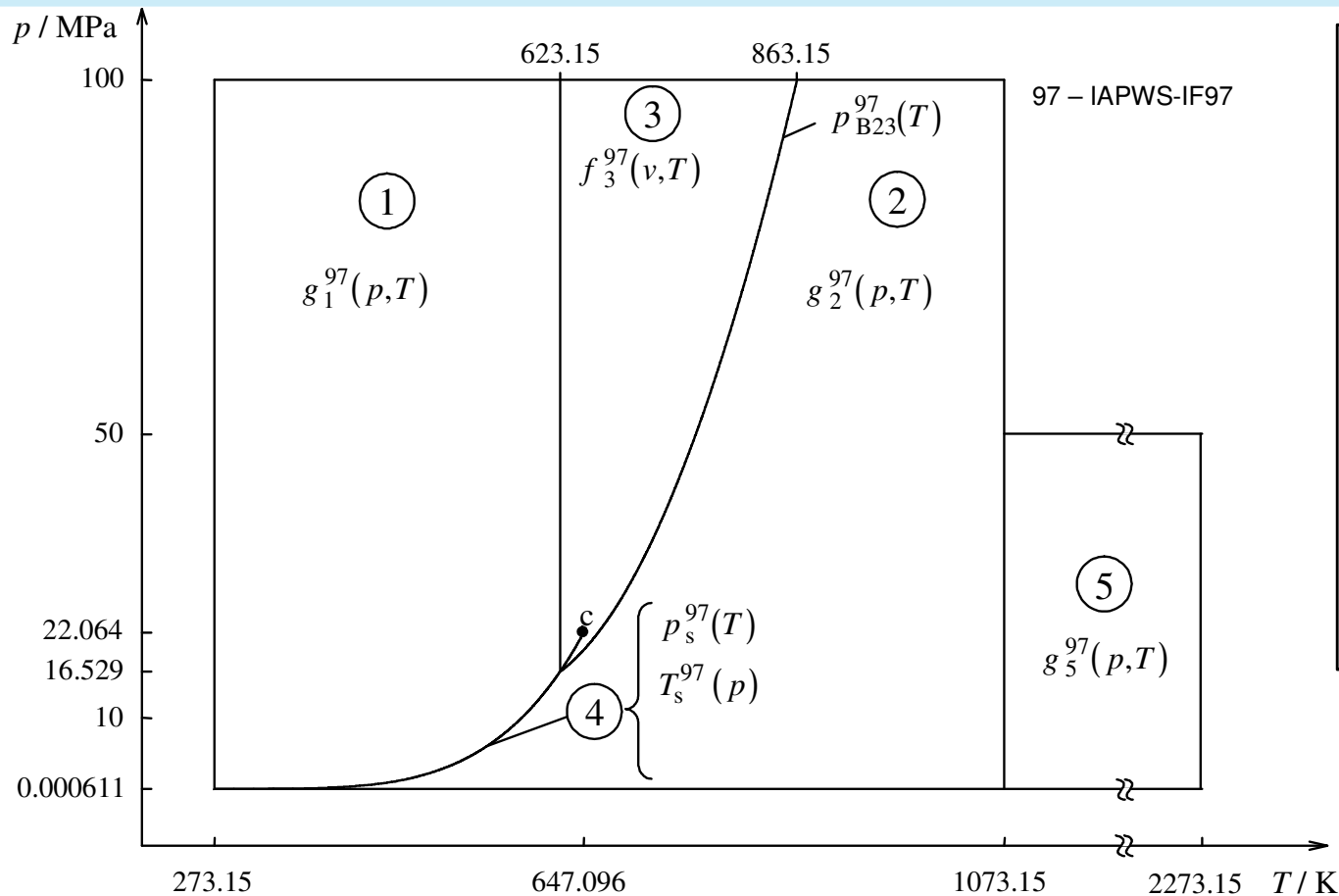
$$\Delta = \theta^2 + B_i \cdot [(\delta - 1)^2]^{a_i} \quad \theta = (1 - \tau) + A_i \cdot [(\delta - 1)^2]^{\frac{1}{2 \cdot \beta_i}} \quad \psi = \exp[-C_i \cdot (\delta - 1)^2 - D_i \cdot (\tau - 1)^2]$$

- Represents the measurement data it is based on to within their uncertainties
- Contains numerous computationally intensive terms
- Property functions of  $(v, u)$  and  $(p, h)$  need to be calculated by iteration

 **Computing speed is insufficient for extensive process simulations and needs to be accelerated by factors > 100...1000 to meet the requirements.**

# Available IAPWS-Formulations for Water and Steam

## Industrial Formulation IAPWS-IF97



Region 2:

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

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

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

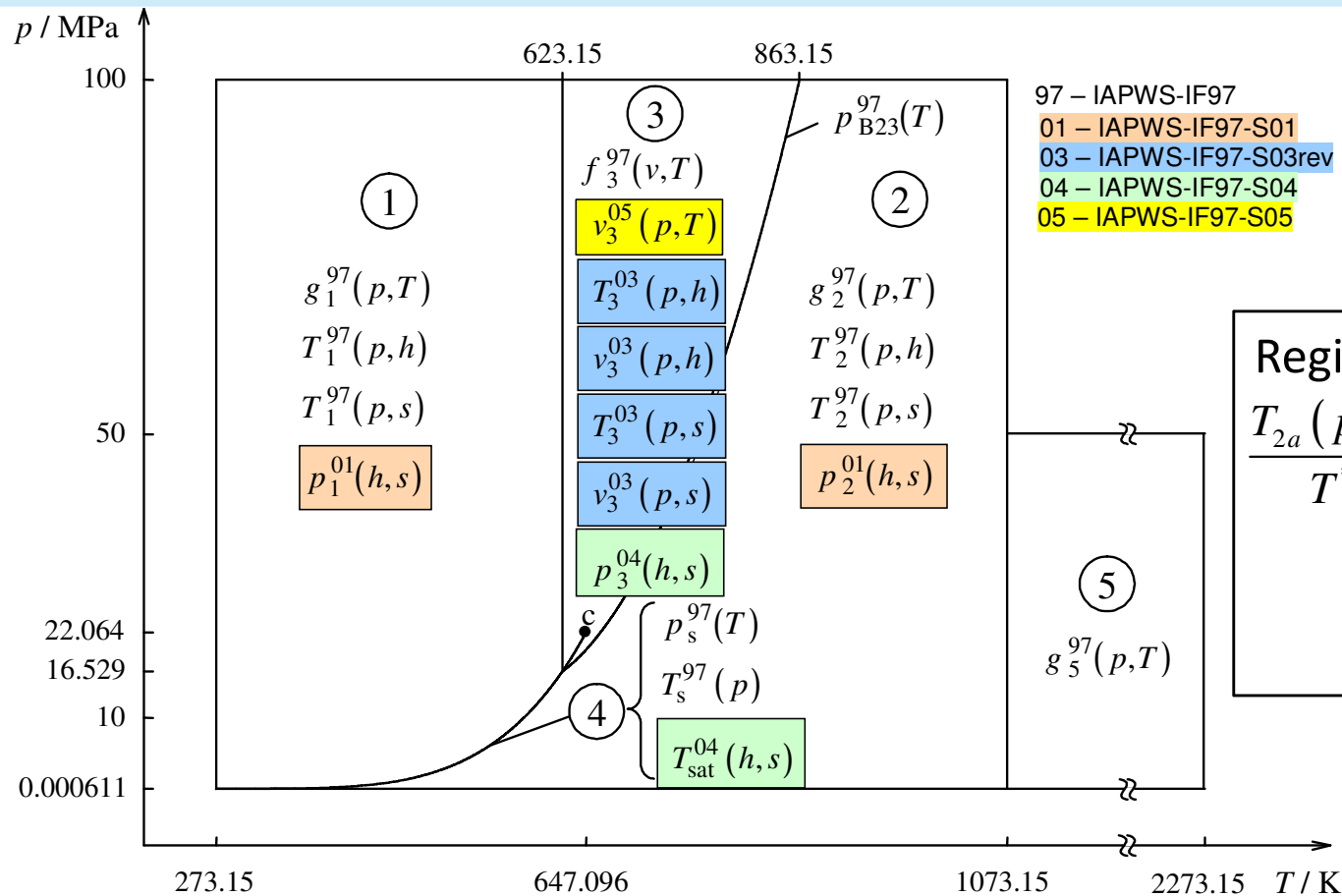
$$\gamma^r(\pi, \tau) = \ln \pi + \sum_{i=1}^{43} n_i \pi^{L_i} (\tau - 0.5)^{J_i}$$

- Basic equations are optimized for computing speed
- Accuracy is sufficient for industrial use
- Property functions of  $(v, u)$  need to be calculated by iteration

➡ Even IAPWS-IF97 is too slow for CFD simulations.

# Available IAPWS-Formulations for Water and Steam

## Industrial Formulation IAPWS-IF97 – Backward Equations



Region 2:

$$\frac{T_{2a}(p, h)}{T^*} = \theta_{2a}(\pi, \eta) = \sum_{i=1}^{34} n_i \pi^{I_i} (\eta - 2.1)^{J_i}$$

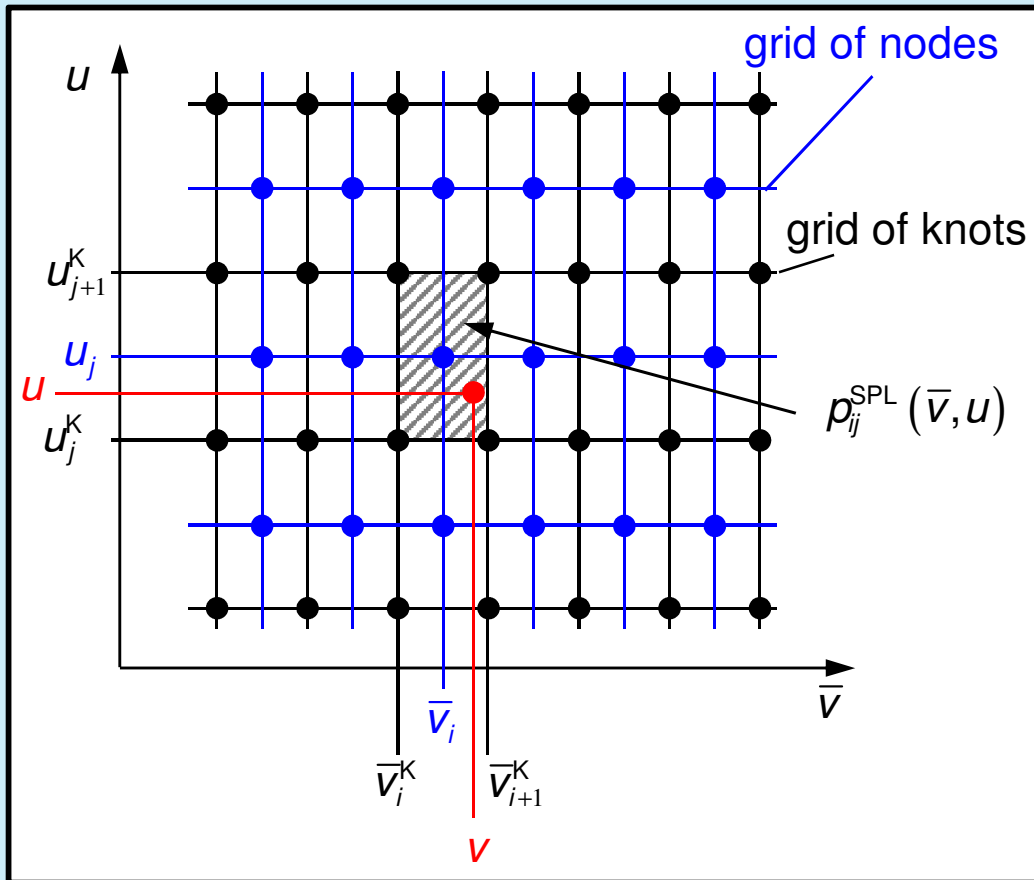
$$\pi = \frac{p}{p^*} \quad \eta = \frac{h}{h^*}$$

- Numerical consistency of backward equations is not sufficient for small spatial and time steps in CFD calculations or the simulation of transient processes in heat-cycles  
 → inverse functions need to be calculated from the basic equations by iteration

➡ Backward equations are not an option for CFD and the simulation of transient processes.

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

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



## ■ Generation of a rectangular grid of nodes:

- each node is calculated from the underlying equation of state:

$$p_{i,j}(\bar{v}_i, u_j) = p^{\text{EOS}}(\bar{v}_i, u_j)$$

## ■ Variable transformation: $v \rightarrow \bar{v}$

- enhance accuracy
- transform the range of state

## ■ Cell definition in the grid of knots:

- spline polynomial:

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

- intersects the inner node
- continuous function and first derivatives

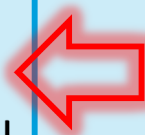
## ■ Optimization for:

- 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:

- transformation of  $v$
- cell  $(i, j)$  determination
- computation of the spline polynomial



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

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

Forward spline function: 
$$p_{ij}^{\text{SPL}}(\bar{v}, u) = \sum_{k=1}^3 \sum_{l=1}^3 a_{ijkl} (\bar{v} - \bar{v}_i)^{k-1} (u - u_j)^{l-1}$$

Inverse spline function: 
$$u_{ij}^{\text{INV}}(p, \bar{v}) = \frac{(-B \pm \sqrt{B^2 - 4AC})}{2A} + u_j$$

where  $A = a_{ij13} + \Delta\bar{v}_i (a_{ij23} + a_{ij33}\Delta\bar{v}_i)$

$$B = a_{ij12} + \Delta\bar{v}_i (a_{ij22} + a_{ij32}\Delta\bar{v}_i)$$

$$C = a_{ij11} + \Delta\bar{v}_i (a_{ij21} + a_{ij31}\Delta\bar{v}_i) - p$$

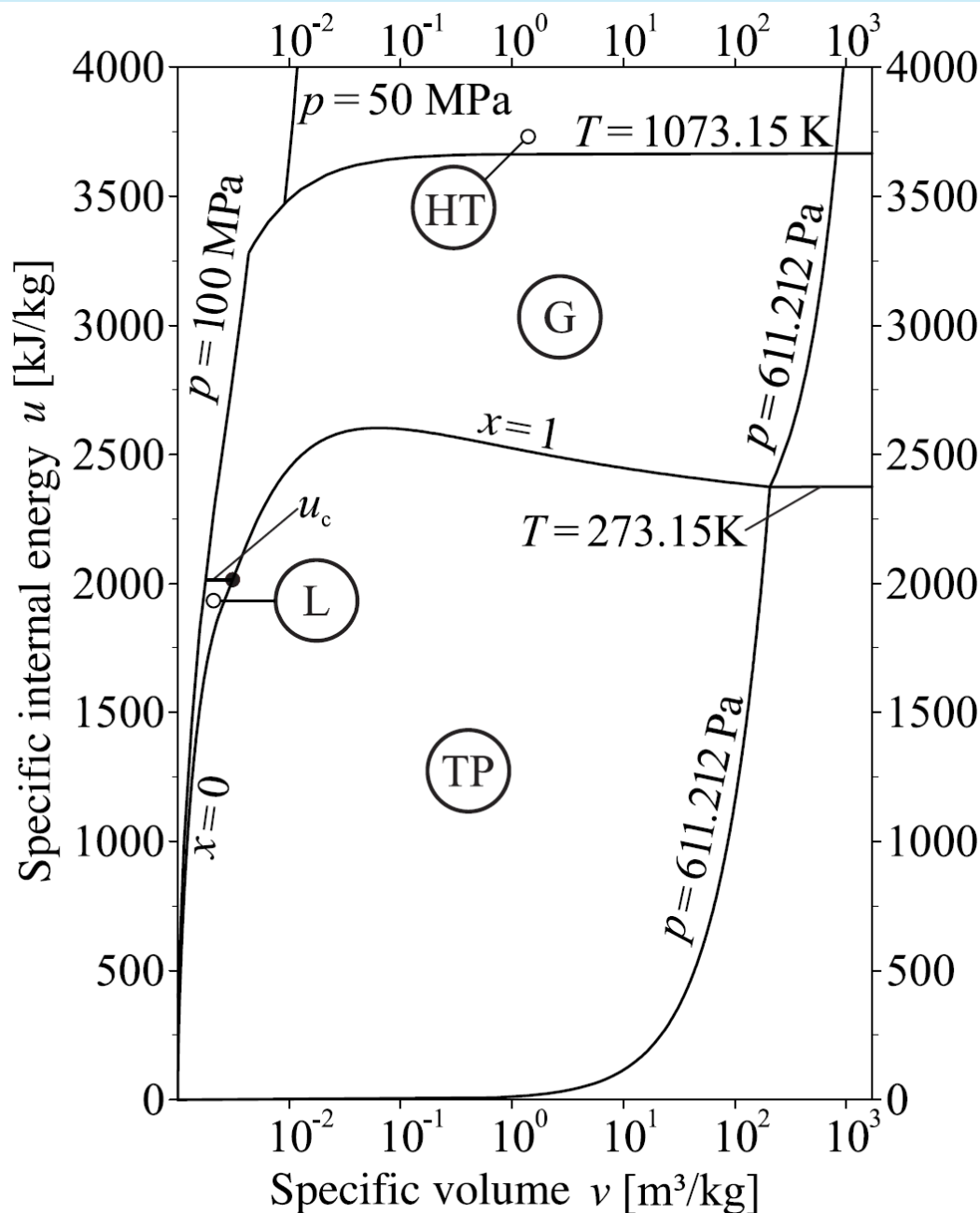
and  $\Delta\bar{v}_i = (\bar{v} - \bar{v}_i)$

$$(\pm) = \text{sign}(B)$$

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

# SBTL Functions of $(v,u)$ and Inverse Functions of $(p,v)$ and $(u,s)$ Based on IAPWS-IF97

Range of validity:



Regions:

L – liquid region

G – gas region

$$273.15 \text{ K} \leq T \leq 1073.15 \text{ K}$$

$$0.611212 \text{ kPa} \leq p \leq 100 \text{ MPa}$$

HT – high-temperature region

$$1073.15 \text{ K} \leq T \leq 2273.15 \text{ K}$$

$$0.611212 \text{ kPa} \leq p \leq 50 \text{ MPa}$$

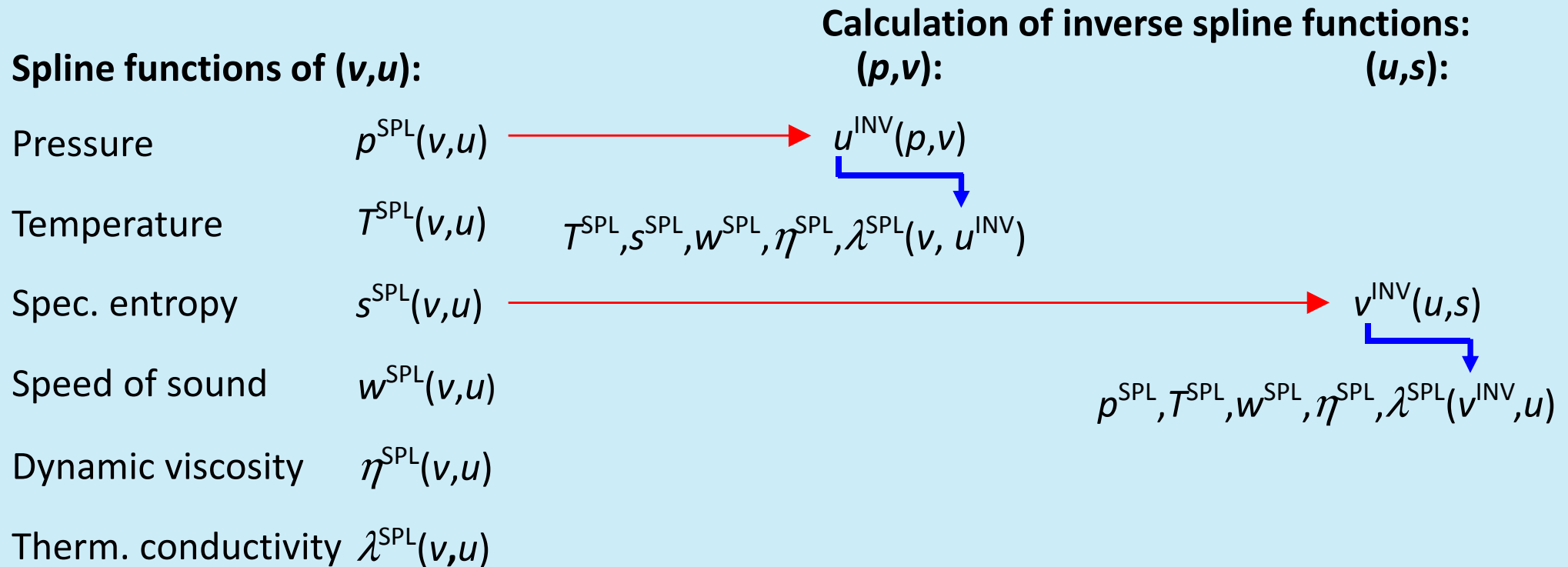
TP – two-phase region

$$273.15 \text{ K} \leq T \leq 647.096 \text{ K}$$

**The Guideline also contains:**

- **SBTL functions for the metastable vapor region**
- **SBTL functions based on IAPWS-95**

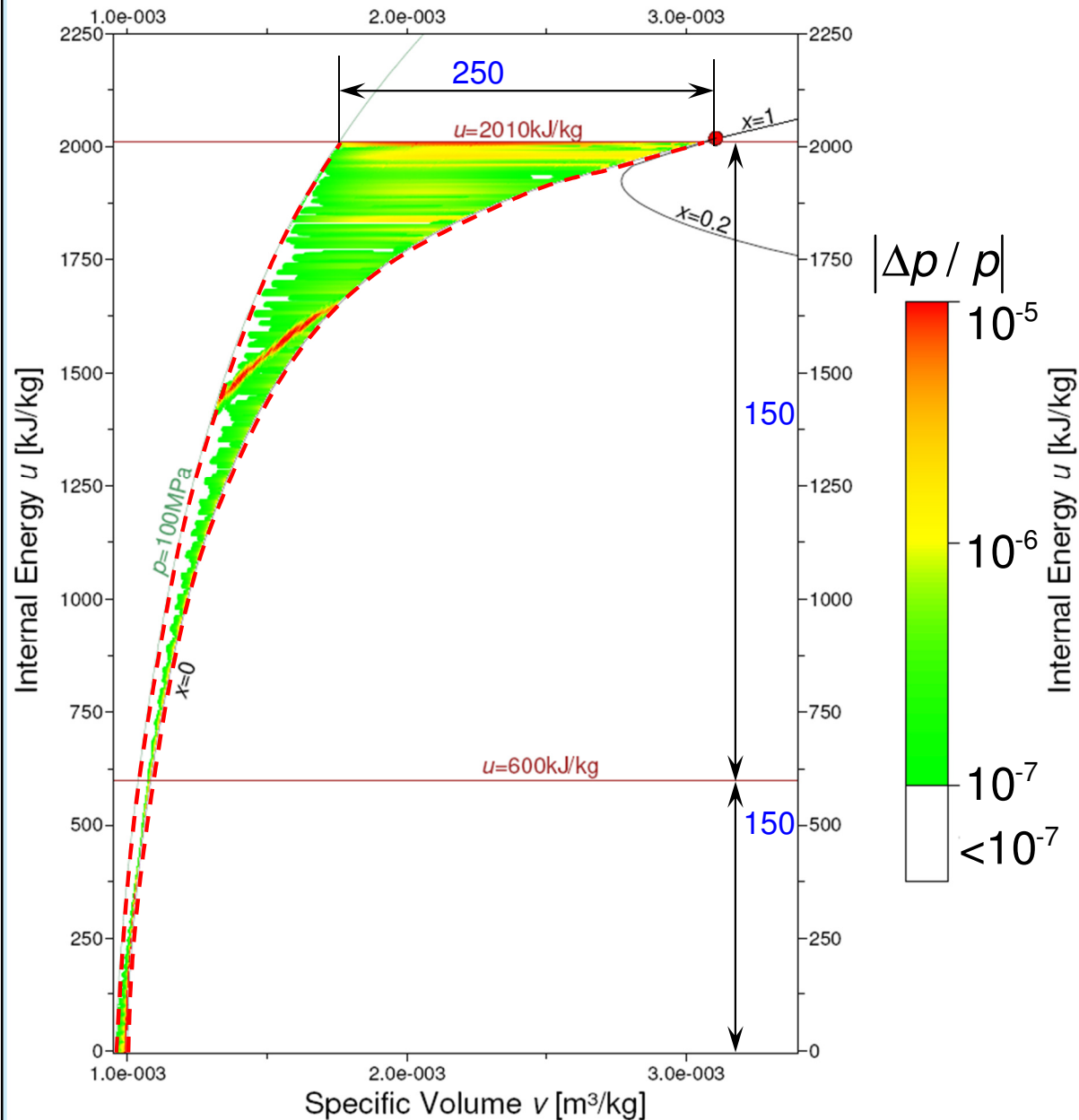
# SBTL Functions of $(v,u)$ and Inverse Functions of $(p,v)$ and $(u,s)$ Based on IAPWS-IF97



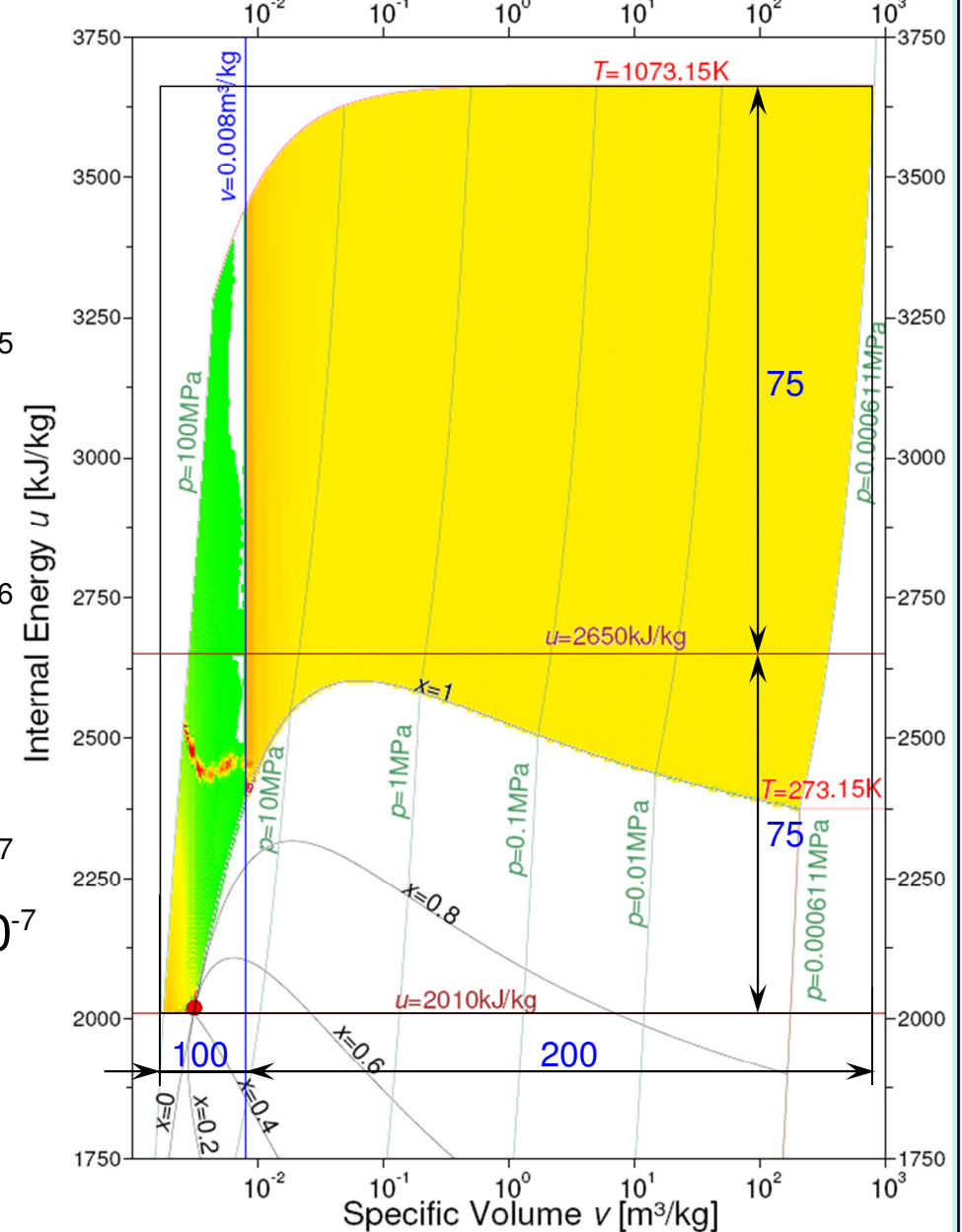
- All thermodynamic and transport properties including derivatives and backward functions are calculated without iterations.
- Forward and backward functions are calculated with complete numerical consistency.

# SBTL Functions $p(v,u)$ – Deviations from IAPWS-IF97

→ Spline function  $p_L(v,u)$ :



→ Spline function  $p_G(v,u)$ :



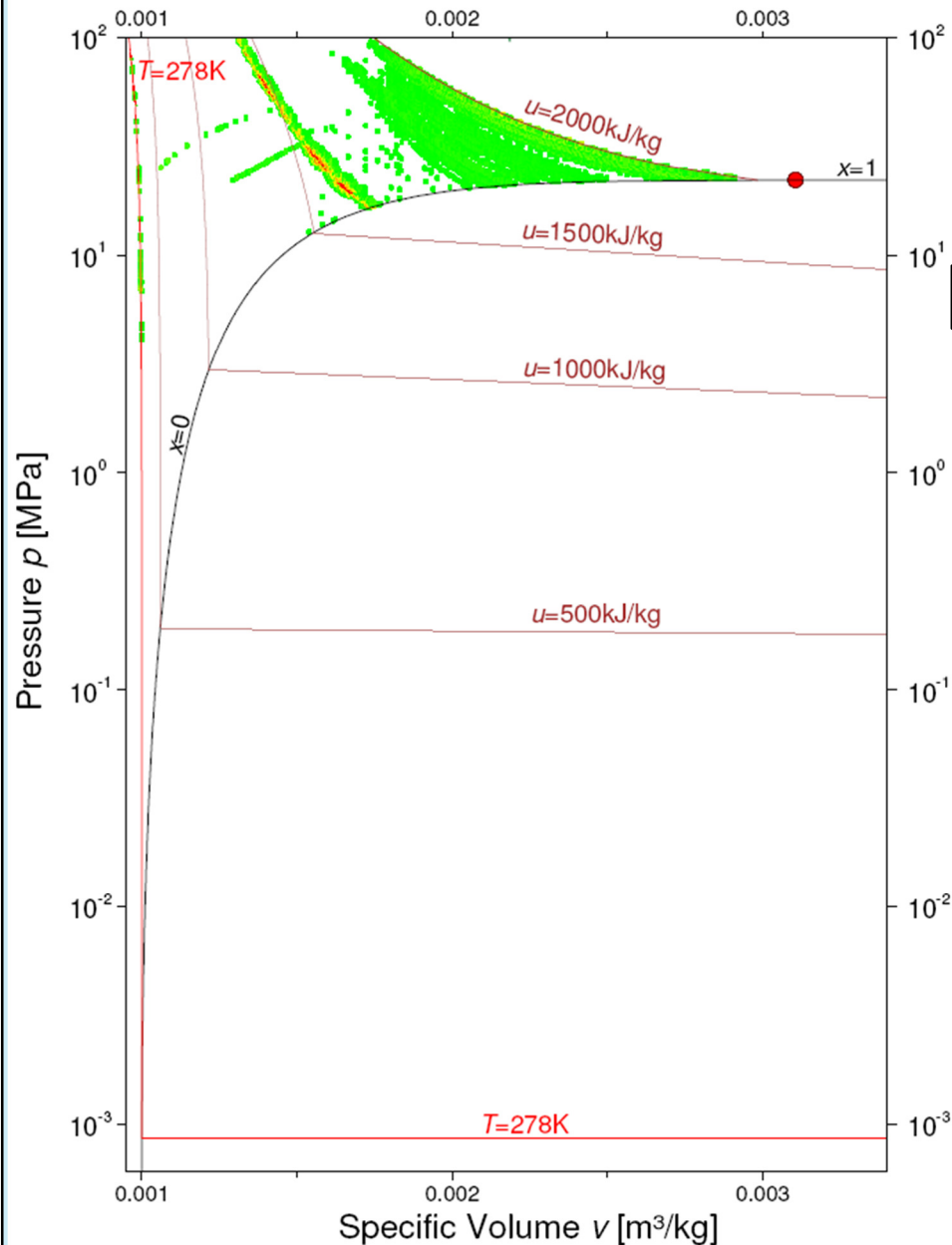
Transformations:

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

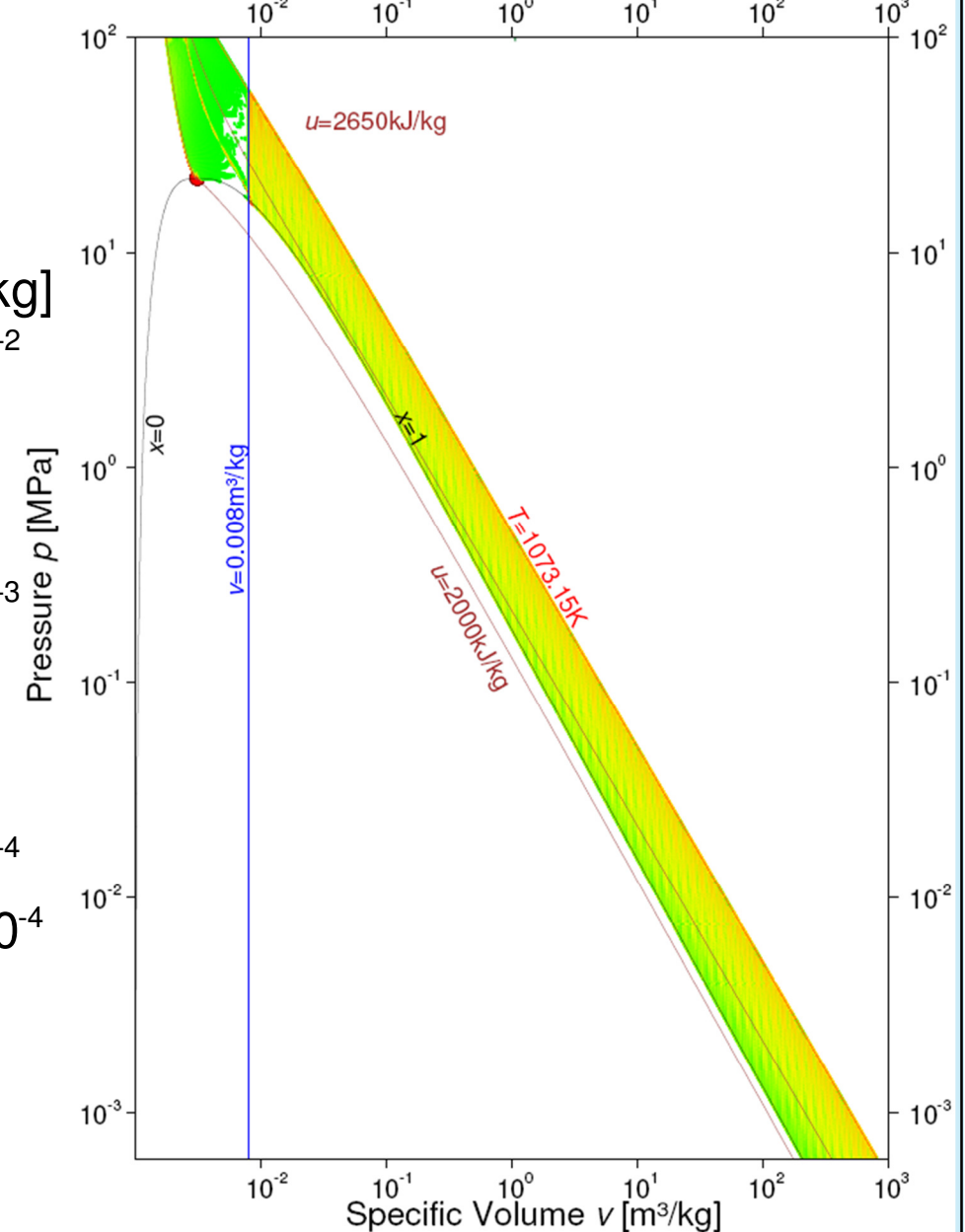
$\bar{v} = \ln(v)$

# Inverse Functions $u(p,v)$ – Deviations from IAPWS-IF97

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



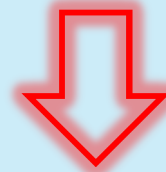
→ Inverse spline function  $u_G(p,v)$ :



➤ Inverse spline functions are numerically consistent with their forward spline functions.

# SBTL Functions of $(v,u)$ and Inverse Functions of $(p,v)$ and $(u,s)$ – Deviations from IAPWS-IF97

SBTL function		Max. deviation (liquid phase)	Max. deviation (vapor phase)
$p(v,u)$	$p \leq 2.5 \text{ MPa}$	$ \Delta p / p  < 0.12 \%$	$ \Delta p / p  < 0.001 \%$
	$p > 2.5 \text{ MPa}$	$ \Delta p  < 0.6 \text{ kPa}$	
$T(v,u)$		$ \Delta T  < 1 \text{ mK}$	$ \Delta T  < 1 \text{ mK}$
$s(v,u)$		$ \Delta s  < 10^{-6} \text{ kJ kg}^{-1} \text{ K}^{-1}$	$ \Delta s  < 10^{-6} \text{ kJ kg}^{-1} \text{ K}^{-1}$
$w(v,u)$		$ \Delta w / w  < 0.001 \%$	$ \Delta w / w  < 0.001 \%$
$\eta(v,u)$		$ \Delta \eta / \eta  < 0.001 \%$	$ \Delta \eta / \eta  < 0.001 \%$



- **Spline-based property functions reproduce the industrial standard IAPWS-IF97 with high accuracy.**
- **Differences between the results of process simulations using the SBTL method and those obtained through the use of IAPWS-IF97 are negligible.**

# 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 (vapor)	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

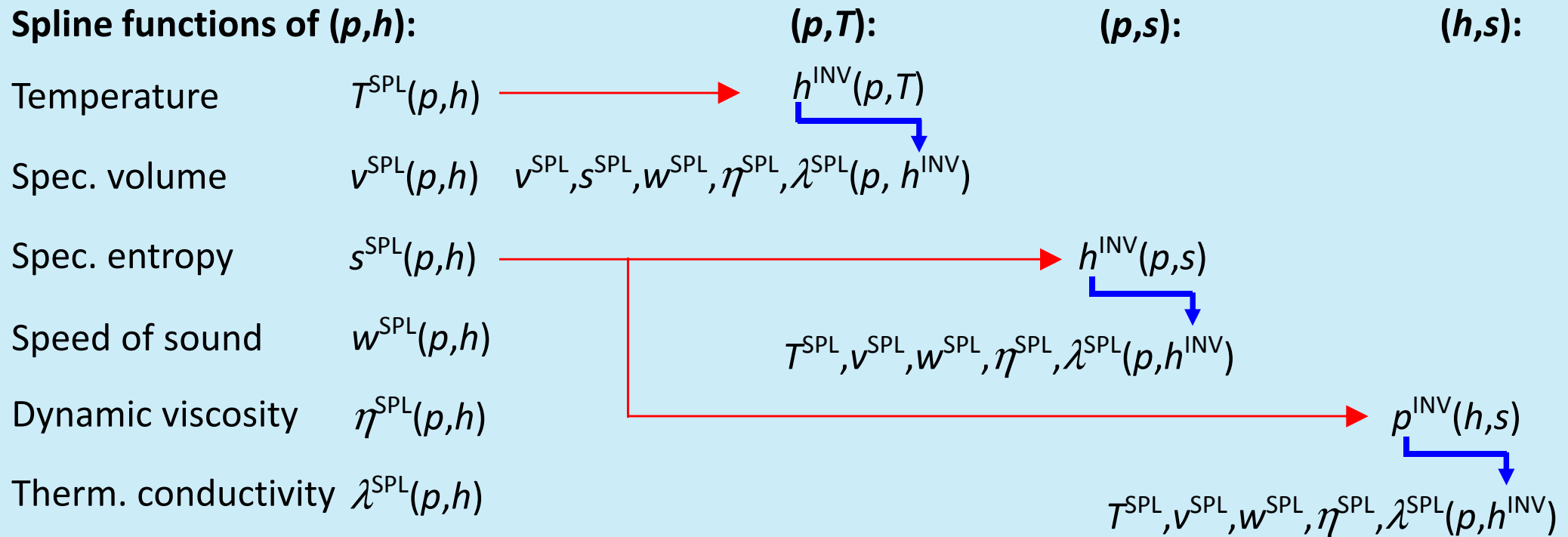
➤ **Computing time for region determination is included in these values.**

**Processor:** Intel Xeon – 3.2GHz

**Operating system:** Windows7 (32 Bit) ➤ **Computing times are reduced by factors up to 300 (500)!**

**Compiler:** Intel Composer XE 2011

# SBTL Functions of $(p,h)$ and Inverse Functions of $(p,T)$ , $(p,s)$ , and $(h,s)$ Based on IAPWS-IF97



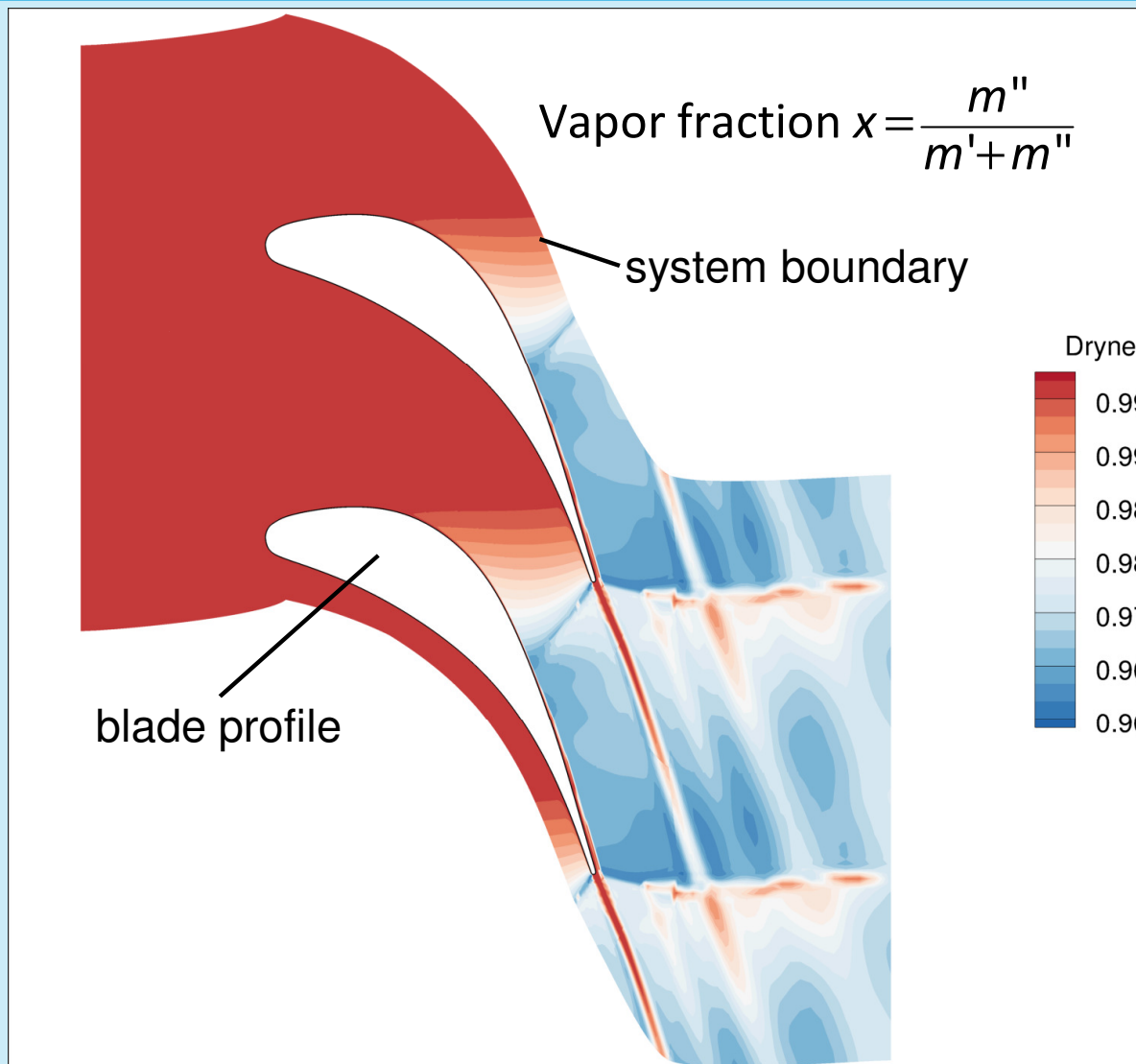
## Deviations from IAPWS-IF97:

SBTL function	Max. deviation
$T(p,h)$	$ \Delta T  < 1 \text{ mK}$
$v(p,h)$	$ \Delta v / v  < 10^{-5}$
$s(p,h)$	$ \Delta s  < 10^{-6} \text{ kJ kg}^{-1} \text{ K}^{-1}$
$w(p,h)$	$ \Delta w / w  < 10^{-5}$
$\eta(p,h)$	$ \Delta \eta / \eta  < 10^{-5}$

## The Guideline contains:

- **SBTL functions for the metastable vapor region**
- **SBTL functions based on IAPWS-95**

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



German Aerospace Center (DLR)  
Institute of Propulsion Technology  
Numerical Methods,  
Cologne, Germany

**CFD-Software TRACE (DLR)**

## Inlet conditions:

- Total pressure: 41.7 kPa
- Total temperature: 357.5 K  
( $\Delta T_s = +7.5$  K)

## Outlet conditions:

- Static pressure: 20.6 kPa

## Assumptions:

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

- In comparison to simulations with IAPWS-IF97, the computing times are reduced by factors of 6 - 10 through the use of the SBTL method.
- With regard to simulations with the ideal-gas model, the computing times are increased by a factor of 1.4 only.

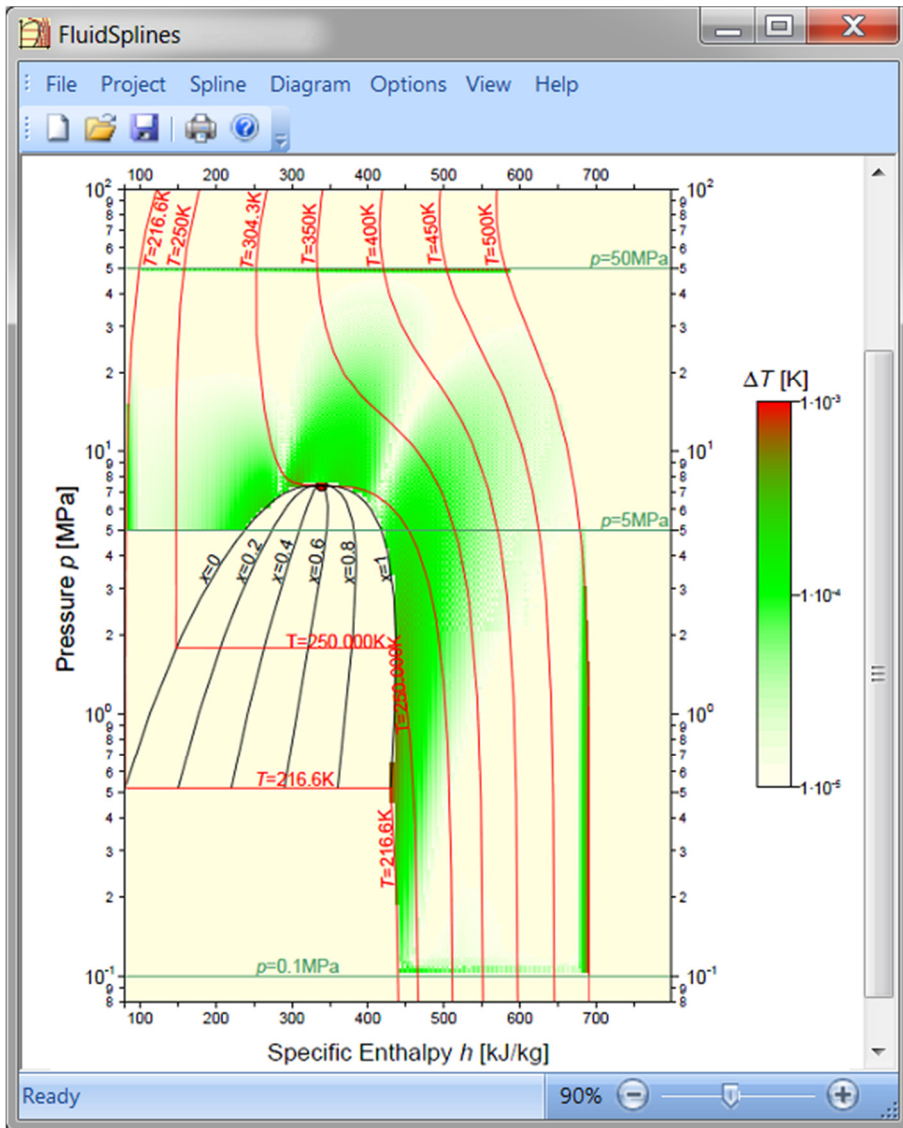
# Application of the SBTL Method in Other Software Products

- **RELAP-7** – Idaho National Laboratory (INL)  
international reference code for  
nuclear-reactor system safety analysis
  - SBTL functions of  $(v,u)$  based on IAPWS-95  
(incl. metastable liquid/vapor)
  
- **DYNAPLANT** – SIEMENS  
simulation of non-stationary processes in power plants
  - SBTL functions of  $(v,h)$  based on IAPWS-IF97
  
- **KRAWAL** – SIEMENS  
heat-cycle calculations for power plant design
  - SBTL functions of  $(p,h)$  based on IAPWS-IF97
  
- **EBSILON Professional** – STEAG Energy Services  
commercial heat-cycle simulation software
  - SBTL functions of  $(p,h)$  based on IAPWS-IF97

# Generation of SBTL Functions for Specific Demands

## FluidSplines

Software for generating  
spline-based property functions



## Input:

(Thermodynamic Properties)

REFPROP<sup>©</sup>

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) – a supplement to existing standards:**
  - Reproduces existing standards with high accuracy at high computing speed
  - Inverse spline functions are numerically consistent with their forward functions
  - Property functions and their first derivatives are continuous
- **SBTL functions based on IAPWS-IF97 and IAPWS-95:**
  - Property functions of IAPWS Standards are reproduced with an accuracy of 10 – 100 ppm
  - Computing speeds are considerably increased  
(SBTL functions of  $(v,u)$  up to 300 times faster than IAPWS-IF97)
- **Applicability in Computational Fluid Dynamics (CFD) has been demonstrated**
  - 6-10 times faster than simulations with IAPWS-IF97
  - Enables consideration of the real fluid behavior with high accuracy
  - Only 40% slower than simulations with the ideal gas model
- **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

# Summary

## **The International Association for the Properties of Water and Steam**

Stockholm, Sweden

July 2015

### **Guideline on the Fast Calculation of Steam and Water Properties with the Spline-Based Table Look-Up Method (SBTL)**

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# **Thank you for your attention!**