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Fast and Accurate Calculation of Thermodynamic Properties Using a Spline-Based Table Look-Up Method

Project of the International Association for the Properties of Water and Steam (IAPWS)
Task Group “CFD Steam Property Formulation”

Outline:

- Requirements for Property Calculations in CFD - Simulations
- Possible Algorithms for Property Calculations in CFD
- Fundamentals of a Spline-Based Table Look-Up Method
- Property Calculations for Water and Steam in CFD-Simulations
- Computing Time Comparisons to Tabular Taylor Series Expansion Method (TTSE)
- FluidSplines – a Tool to Generate Spline-Based Property Functions
- Summary

IAPWS Meeting, Boulder 2012

Requirements for Property Calculations in CFD - Simulations

The development of new technologies for power generation requires extensive process simulations:

- **Integration of wind and solar energy into the power grid requires flexible control of conventional power plants**

Simulation of non stationary processes

- **Development and optimization of heat cycle components**

Flow analysis with Computational Fluid Dynamics (CFD)

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Requirements for Property Calculations:

- **High accuracy (comparable to a fundamental equation of state)**
- **High computing speed (>100 times faster than a fundamental equation of state)**
- **High numerical consistency of forward and backward functions**
- **Continuous functions and first derivatives**

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IAPWS Task Group "CFD Steam Property Formulation"

Possible Algorithms for Property Calculations in CFD

Problem:

- CFD: calculation from internal energy u and specific volume v
- IAPWS-IF97:
  - no backward equations $z = f(u,v)$ available
  - calculation in single phase region from (p,T)

  ⇩

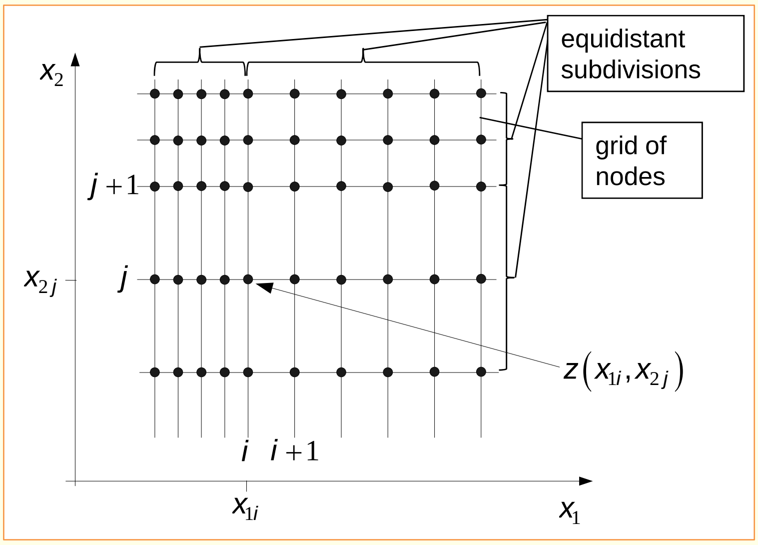
  - two-dimensional iteration for $z = f(u,v)$ required
  - low computing speed

Possible Algorithms:

- Development of Backward Equations $z = f(u,v)$
  - high efforts
  - computing times comparable to existing backward equations
  - limited numerical consistency to IAPWS-IF97
- Development of a Fundamental Equation $s(u,v)$
  - high efforts
  - computing times comparable to fundamental equations of IAPWS-IF97
  - values not in agreement with IAPWS-IF97
- Application of a Spline-Based Table Look-up Method
  - very high computing speed
  - complete numerical consistency of forward and backward functions
  - existing standards can be reproduced with high accuracy

Fundamentals of a Spline-Based Table Look-Up Method

Generation of a spline-function $z^{SPL}(x_1,x_2)$ from an existing equation of state $z^{EOS}(x_1,x_2)$:



- Generation of a grid of nodes, optimized for:
  - required accuracy
  - maximal computing speed
  - minimal amount of data
- Calculation of node-values from equation of state
- Calculation of all spline-coefficients for all cells

$$z_{ij}^{SPL}(x_1,x_2) = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ijkl}\,(x_1 - x_{1i})^{k-1}(x_2 - x_{2j})^{l-1}$$

To provide spline-based functions for property calculations:

- save grid of nodes and spline-coefficients
- generate optimized source-code for the property function $z^{SPL}(x_1,x_2)$

⇨ **Application of spline-functions in CFD and other extensive simulations**

Fundamentals of a Spline-Based Table Look-Up Method

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

$$z_{ij}^{\mathrm{SPL}}\left(x_1,x_2\right)=\sum_{k=1}^{3}\sum_{l=1}^{3}a_{ijkl}\left(x_1-x_{1i}\right)^{k-1}\left(x_2-x_{2j}\right)^{l-1}$$

$$\Rightarrow\quad x_{1,ij}^{\mathrm{INV}}\left(z,x_2\right)=\frac{\left(-B\pm\sqrt{B^2-4AC}\right)}{2A}+x_{1i}$$

in which

$$A=a_{ij31}+\Delta x_{2j}\left(a_{ij32}+a_{ij33}\Delta x_{2j}\right)$$

$$B=a_{ij21}+\Delta x_{2j}\left(a_{ij22}+a_{ij23}\Delta x_{2j}\right)$$

$$C=a_{ij11}+\Delta x_{2j}\left(a_{ij12}+a_{ij13}\Delta x_{2j}\right)-z$$

and

$$\Delta x_{2j}=\left(x_2-x_{2j}\right)$$

⇓

The inverse spline-function $x_{1,ij}^{\mathrm{INV}}\left(z,x_2\right)$ is numerically consistent to the spline-function $z_{ij}^{\mathrm{SPL}}\left(x_1,x_2\right)$.

Property Calculations for Water and Steam in CFD-Simulations

Application of inverse spline-functions (independent variables: *u*,*v*):

→ spline-functions with the variables *u* and *v*: $p^{\mathrm{SPL}}(u,v)$ $T^{\mathrm{SPL}}(u,v)$ $s^{\mathrm{SPL}}(u,v)$ $\eta^{\mathrm{SPL}}(u,v)$ $\lambda^{\mathrm{SPL}}(u,v)$

→ calculation from other pairs of variables using the spline-functions above:

$T,s,u,\eta = \mathrm{f}(p,v)$	$T,v,s,\eta = \mathrm{f}(p,u)$	$p,T,v,\eta = \mathrm{f}(u,s)$
$u = u^{\mathrm{INV}}(p,v)$	$v = v^{\mathrm{INV}}(p,u)$	$v = v^{\mathrm{INV}}(u,s)$
$T = T^{\mathrm{SPL}}(u,v)$	$T = T^{\mathrm{SPL}}(u,v)$	$p = p^{\mathrm{SPL}}(u,v)$
$s = s^{\mathrm{SPL}}(u,v)$	$s = s^{\mathrm{SPL}}(u,v)$	$T = T^{\mathrm{SPL}}(u,v)$
$\eta = \eta^{\mathrm{SPL}}(u,v)$	$\eta = \eta^{\mathrm{SPL}}(u,v)$	$\eta = \eta^{\mathrm{SPL}}(u,v)$

→ inverse spline functions: $u = u^{\mathrm{INV}}(p,v)$, $v = v^{\mathrm{INV}}(p,u)$, $v = v^{\mathrm{INV}}(u,s)$

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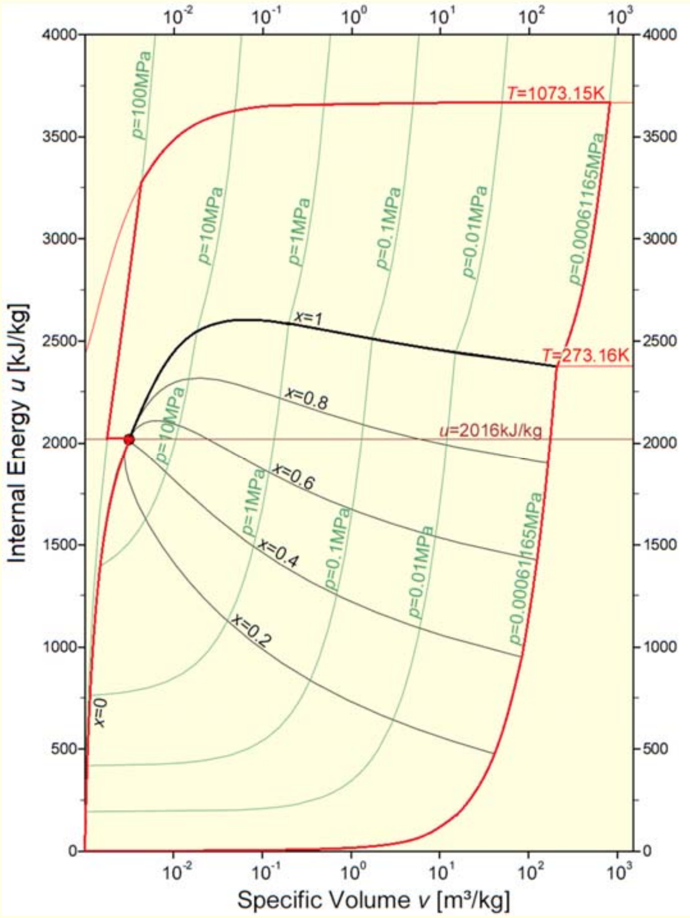
- **All thermodynamic properties, including backward-functions, can be calculated without iterations.**
- **Spline-functions can be calculated with complete numerical consistency.**

Property Calculations for Water and Steam in CFD-Simulations



Required Range of Validity:

Superheated vapor:

0.000612 MPa ≤ p ≤ 100 MPa

273.16 K ≤ T ≤ 1073.15 K

Two-phase region:

273.16 K ≤ T ≤ 647.096 K

0 kg/kg ≤ x ≤ 1 kg/kg

Available Equations of State:

IAPWS-IF97:

Single-phase region: $g(p,T)$

Critical and supercritical region: $f(T,v)$

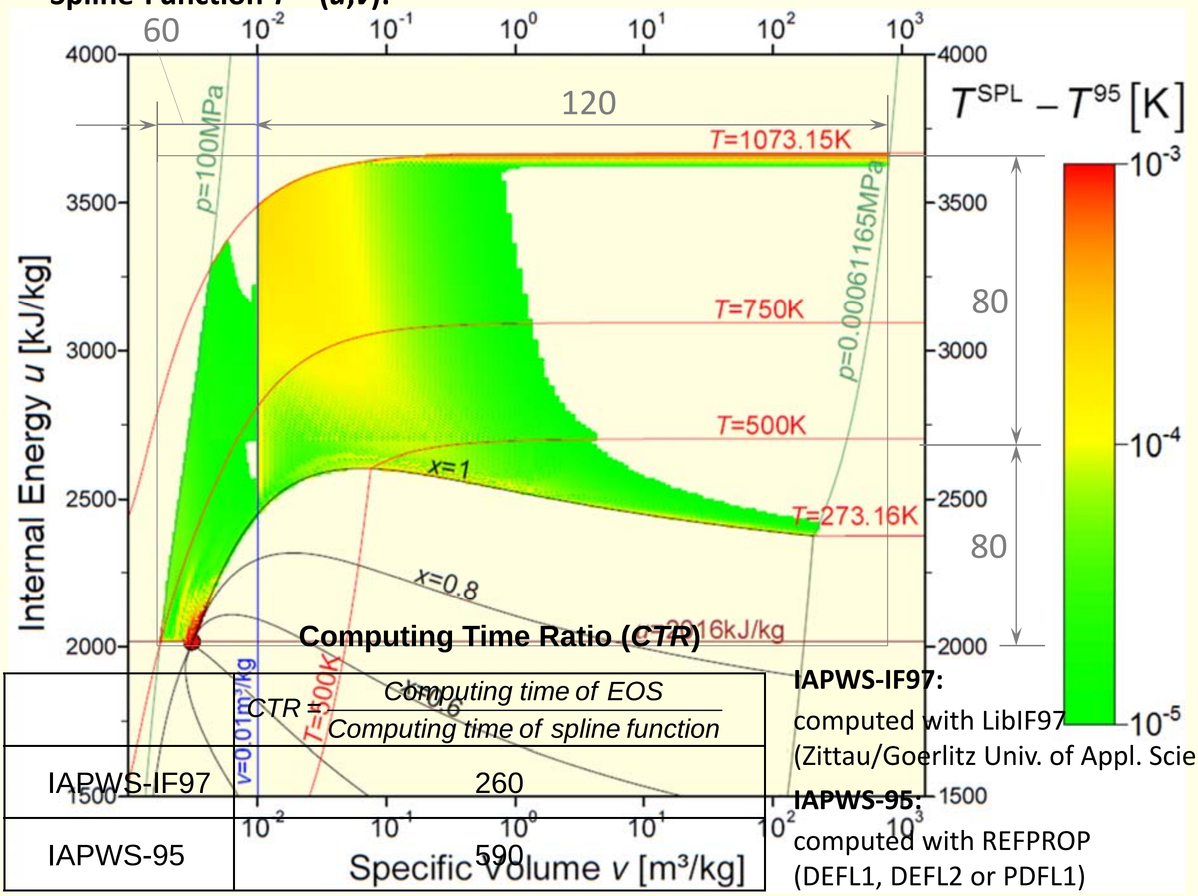
Two-phase region: $p_s(T)$

IAPWS-95:

Helmholtz-equation of state: $f(T,v)$

Property Calculations for Water and Steam in CFD-Simulations

→ **Spline-Function $T^{SPL}(u,v)$:**



Computing Time Ratio (CTR)

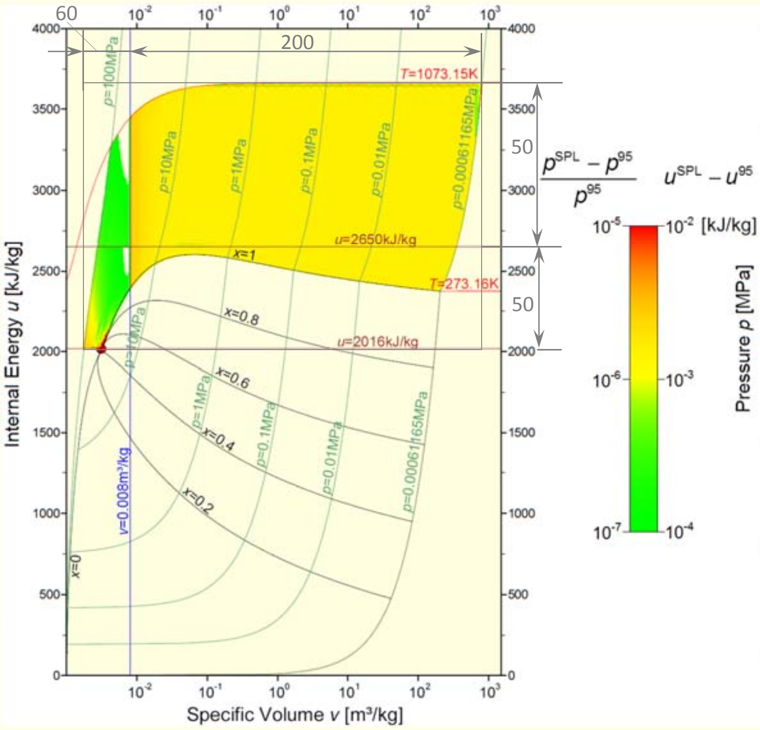
	$CTR = \dfrac{\text{Computing time of EOS}}{\text{Computing time of spline function}}$
IAPWS-IF97	260
IAPWS-95	590

IAPWS-IF97:
computed with LibIF97
(Zittau/Goerlitz Univ. of Appl. Sciences)

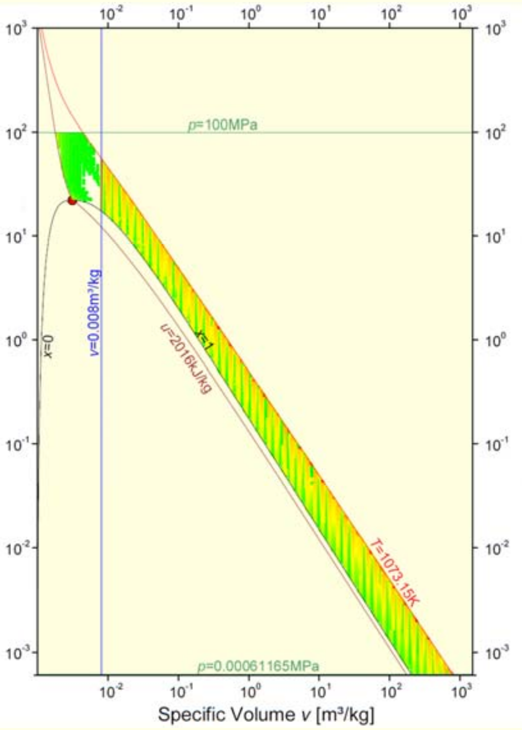
IAPWS-95:
computed with REFPROP
(DEFL1, DEFL2 or PDFL1)

Property Calculations for Water and Steam in CFD-Simulations

→ Spline-Function $p^{SPL}(u,v)$:



→ Inverse Spline-Function $u^{INV}(p,v)$:

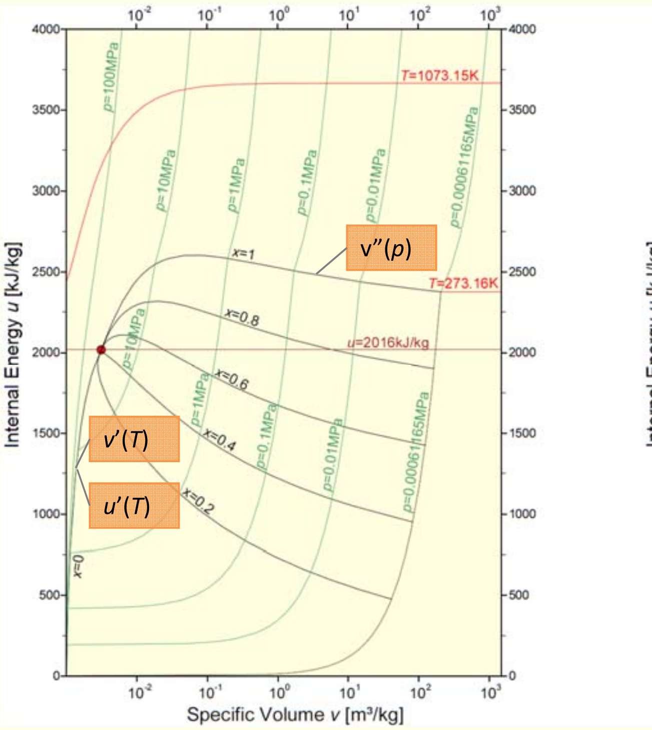


Computing time ratio in comparison to IAPWS-IF97 (IAPWS-95):

***CTR* ≈ 260 (590)** | ***CTR* ≈ 19 (160)**

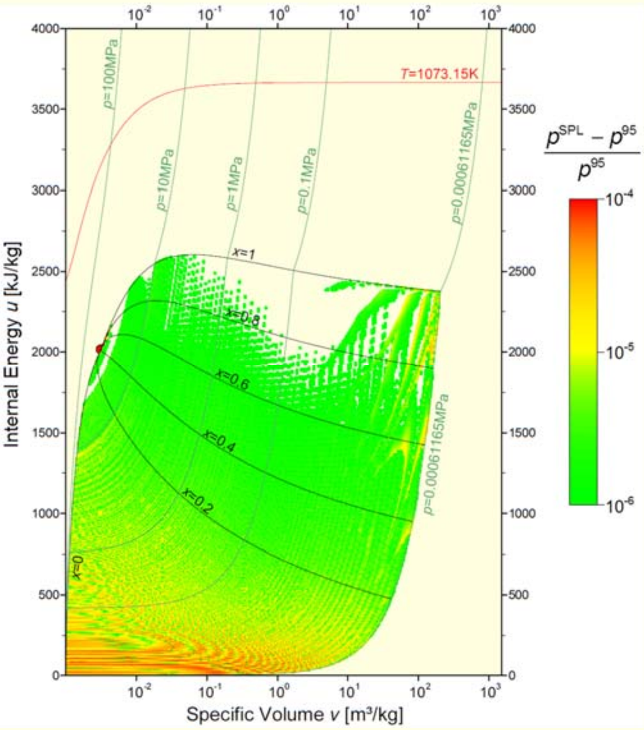
Property Calculations for Water and Steam in CFD-Simulations

→ Auxiliary Functions for Two-Phase Region:



- High numerical consistency at dew curve
- Distinct phase test

→ Saturation Pressure $p_s(u,v)$:

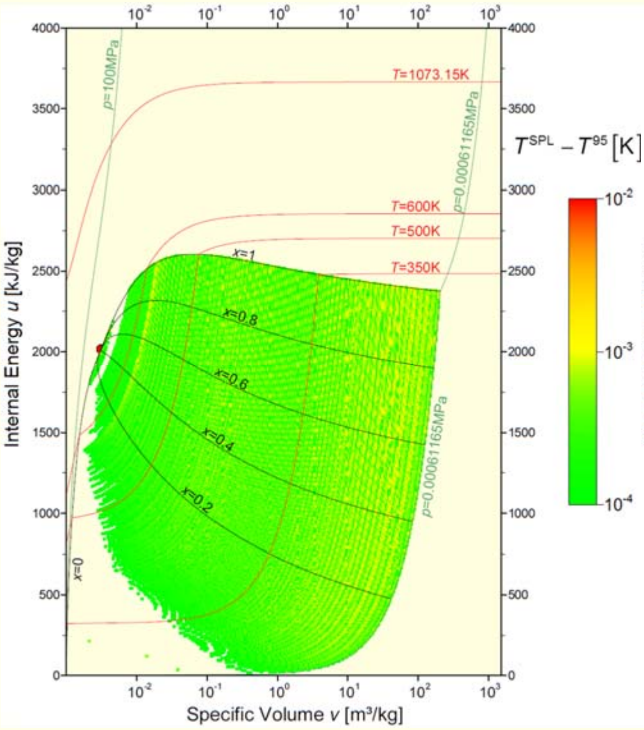


Computing time ratio in comparison to IAPWS-IF97 (IAPWS-95):

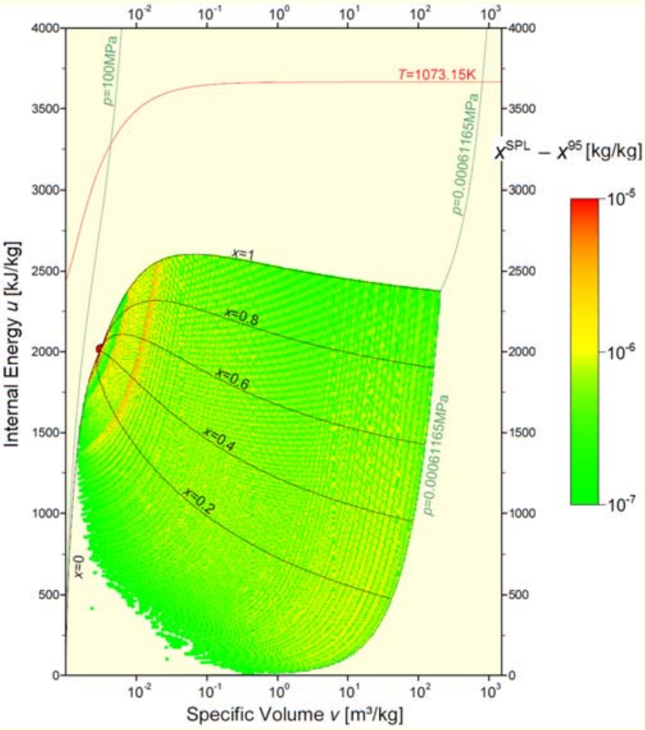
***CTR* ≈ 3 (490)**

Property Calculations for Water and Steam in CFD-Simulations

→ Saturation Temperature $T_s(u,v)$:



→ Vapor Fraction $x(u,v)$:



Computing time ratio in comparison to IAPWS-IF97 (IAPWS-95):

***CTR* ≈ 3 (490)**

Computing Time Comparisons to TTSE - $T(p,h)$ in IAPWS-IF97 Region 2

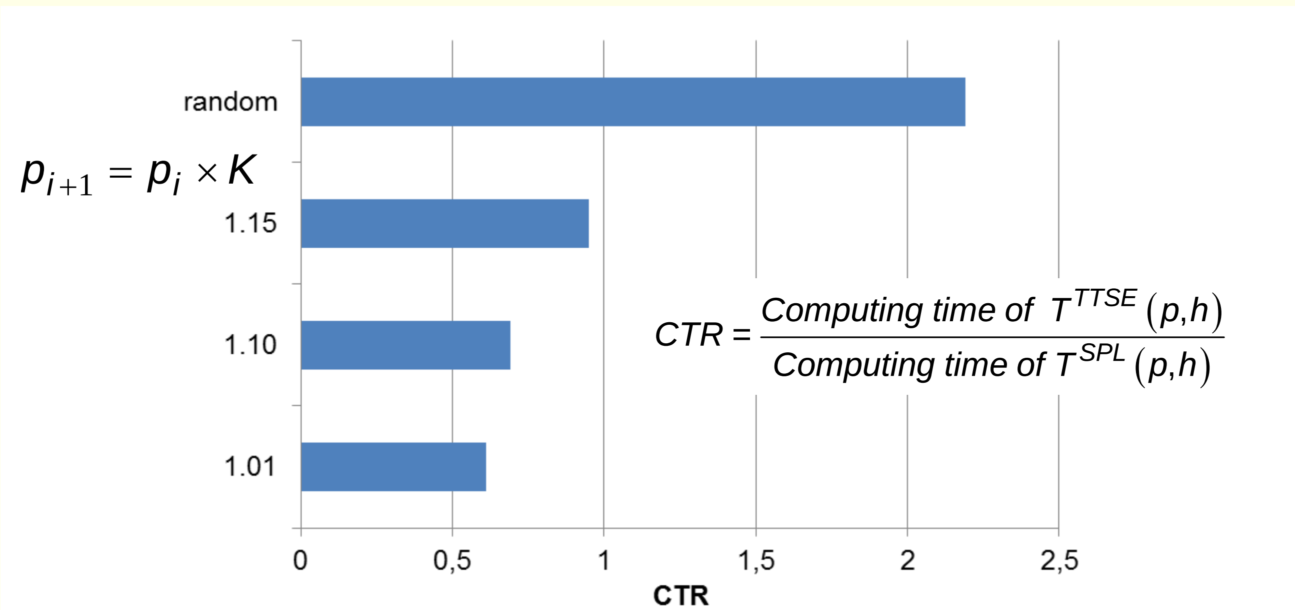
in collaboration with Kiyoshi Miyagawa

Tabular Taylor Series Expansion Method (TTSE)

- $|T^{TTSE}-T^{95}|_{max}$=152mK
- optimized for sequential calls
- discontinuities at cell boundaries

Spline Based Table Look-Up Method

- $|T^{SPL}-T^{95}|_{max}$=2mK
- optimized for random calls
- continuous function
- complete numerical consistency



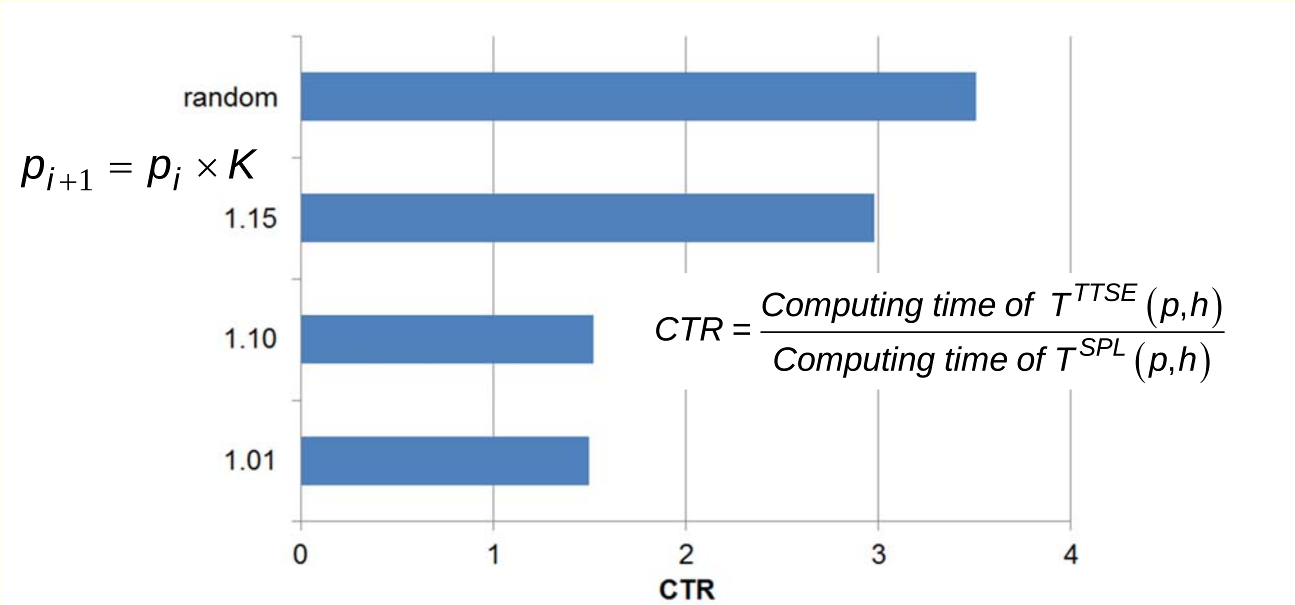
Computing Time Comparisons to TTSE - *T*(*p*,*h*) in IAPWS-IF97 Region 2

Tabular Taylor Series Expansion Method (TTSE)

- $|T^{TTSE}-T^{95}|_{max}$=152mK
- optimized for sequential calls
- discontinuities at cell boundaries

Spline Based Table Look-Up Method

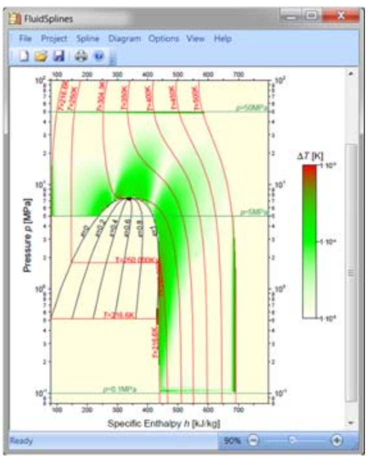
- $|T^{SPL}-T^{95}|_{max}$=152mK
- optimized for sequential calls
- continuous function
- complete numerical consistency



FluidSplines – a Tool to Generate Spline-Based Property Functions

FluidSplines

Software for generating property functions based on spline-interpolation



Generation of Spline-Functions for:

- specified range of validity
- required accuracy

Additional Features:

- generation of inverse spline-functions
- accuracy check
- computing time check

Thermodynamic Properties:

(Database)

REFPROP©

Property-Libraries (Zittau/Goerlitz Univ.)

Output:

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

Application of Property-Functions Based on Spline-Interpolation:

- Computational Fluid Dynamics (CFD)
- extensive heat-cycle calculations (optimization of heat cycles)
- calculation of non-stationary processes
- other applications

Summary

- The Spline-based table look-up method provides high accuracy and high computing speed at the same time.
- Property functions of IAPWS-IF97 or IAPWS-95 are reproduced with an accuracy of 10 ppm - the results of a process simulation will not change.
- The whole range of validity of IAPWS-IF97 can be covered including the wet steam region and the metastable vapor phase.
- Property functions and first derivatives are represented continuously (unlike TTSE).
- Complete numerical consistency of forward and backward functions is realized.
- The Spline-based table look-up method is much faster than the calculation from the basic equations of IAPWS-IF97, and is even faster than the calculation from backward equations or from the TTSE.
- The software tool FluidSplines is available to prepare spline based property functions according to user's requirements (independent variables, range of validity, accuracy).

Requirements of Computational Fluid Dynamics and the calculation of non-stationary processes are fulfilled with this spline based table look-up method.

Thank you for your attention.