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Fast Calculation of Thermodynamic Properties of Water and Steam 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 Process Simulations**
- **Fundamentals of a Spline-Based Table Look-Up Method**
- **Property Calculations for Water and Steam in CFD-Simulations**
- **Application of the Spline based Table Look-up Method in CFD**
- **FluidSplines – a Tool to Generate Spline-Based Property Functions**
- **Summary**

Thermophysical Properties for Technical Thermodynamics, Rostock 2013

Requirements for Property Calculations in Process Simulations

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 in heat cycle calculations**
- **Development and optimization of heat cycle components**
  ⇨ **Flow analysis with Computational Fluid Dynamics (CFD)**

⇩

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**

Requirements for Property Calculations in Process Simulations

Equations of State cannot meet the requirement for high computing speed because:

- **independent variables of Helmholtz-equations are temperature *T* and specific volume *v*,**
  - Heat Cycle Calculations: calculation from pressure *p* and specific enthalpy *h*
  - CFD: calculation from internal energy u and specific volume *v*
  - ➢ **iterative calculation of properties required**
- **equations of state contain numerous terms,**
- **complexity of terms (rational exponents, logarithms, …).**

⇨ **Computing times must be reduced by factors >100…1000 to meet the requirements.**

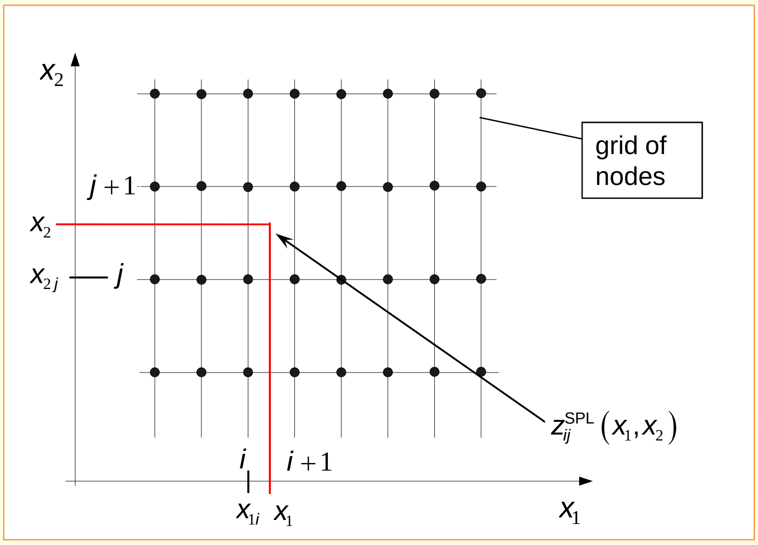
⇩

Application of a Spline-Based Table Look-Up Method to available equations of state is advantageous in extensive process simulations because:

- **results of the equation of state can be reproduced with high accuracy and high computing speed,**
- **spline-functions represent property functions continuously,**
- **backward functions can be calculated with complete numerical consistency.**

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):

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

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

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

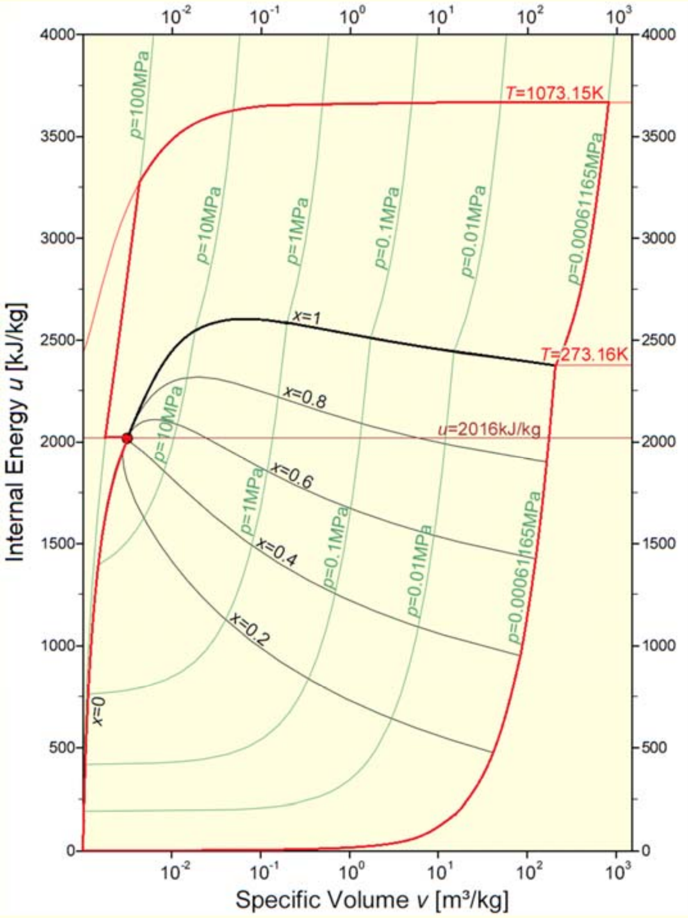
Property Calculations for Water and Steam in CFD-Simulations

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

- **spline-functions with the variables *u* and *v*:** $p^{\text{SPL}}(u,\rho)$, $T^{\text{SPL}}(u,\rho)$, $s^{\text{SPL}}(u,\rho)$, $\eta^{\text{SPL}}(u,\rho)$, $\lambda^{\text{SPL}}(u,\rho)$
- **calculation from other pairs of variables using the spline-functions above:**
  - $T, s, u, \eta = \mathrm{f}(p,\rho)$
  - $T, \rho, s, \eta = \mathrm{f}(p,u)$
  - $p, T, \rho, \eta = \mathrm{f}(u,s)$
- **inverse spline functions:**
  - $u = u^{\text{INV}}(p,\rho)$ → $T = T^{\text{SPL}}(u,\rho)$, $s = s^{\text{SPL}}(u,\rho)$, $\eta = \eta^{\text{SPL}}(u,\rho)$
  - $\rho = \rho^{\text{INV}}(p,u)$ → $T = T^{\text{SPL}}(u,\rho)$, $s = s^{\text{SPL}}(u,\rho)$, $\eta = \eta^{\text{SPL}}(u,\rho)$
  - $\rho = \rho^{\text{INV}}(u,s)$ → $p = p^{\text{SPL}}(u,\rho)$, $T = T^{\text{SPL}}(u,\rho)$, $\eta = \eta^{\text{SPL}}(u,\rho)$

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

Property Calculations for Water and Steam in CFD-Simulations



Required Range of Validity:

Superheated vapor:

$0.000612\ \text{MPa} \le p \le 100\ \text{MPa}$

$273.16\ \text{K} \le T \le 1073.15\ \text{K}$

Two-phase region:

$273.16\ \text{K} \le T \le 647.096\ \text{K}$

$0\ \text{kg/kg} \le x \le 1\ \text{kg/kg}$

Available Equations of State:

IAPWS-IF97:

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

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

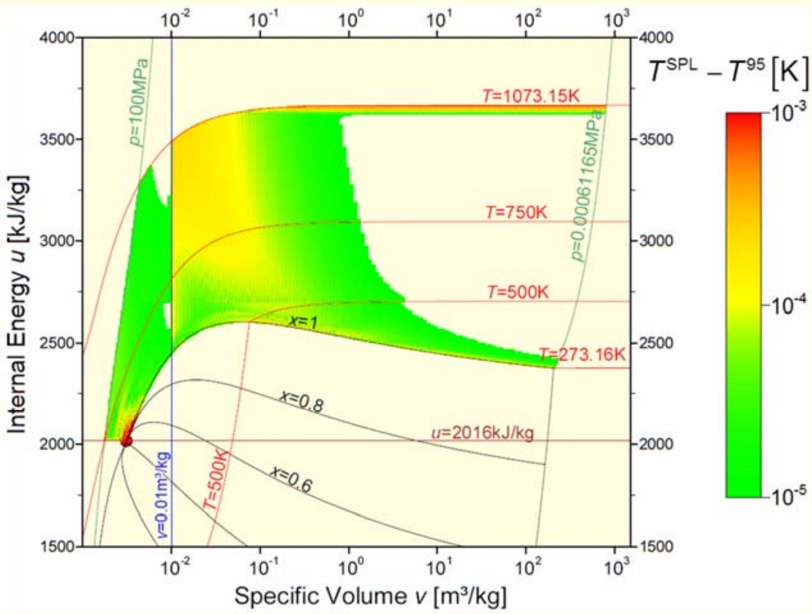
Two-phase region: $p_s(T)$

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)

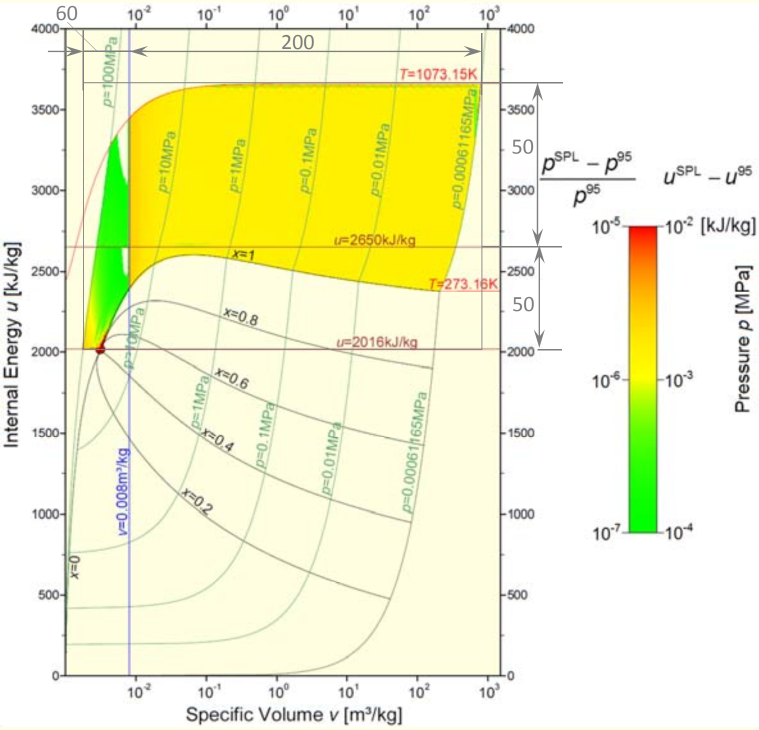
IAPWS-95:

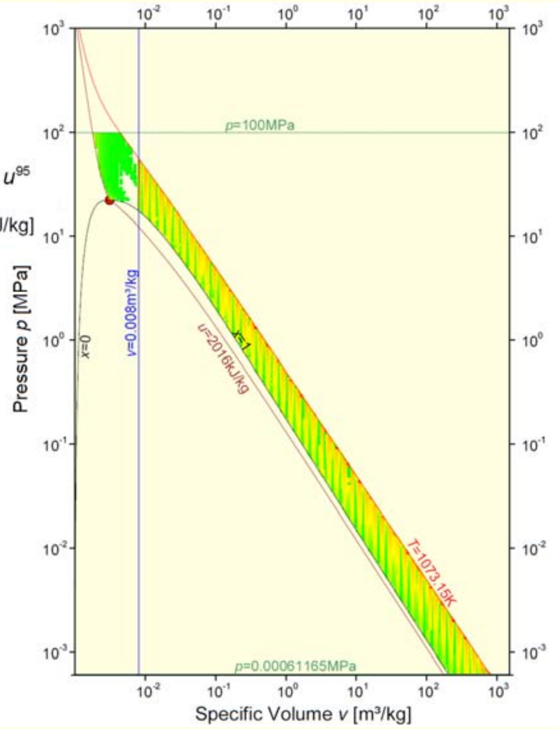
computed with REFPROP (DEFL1, DEFL2 or PDFL1)

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):

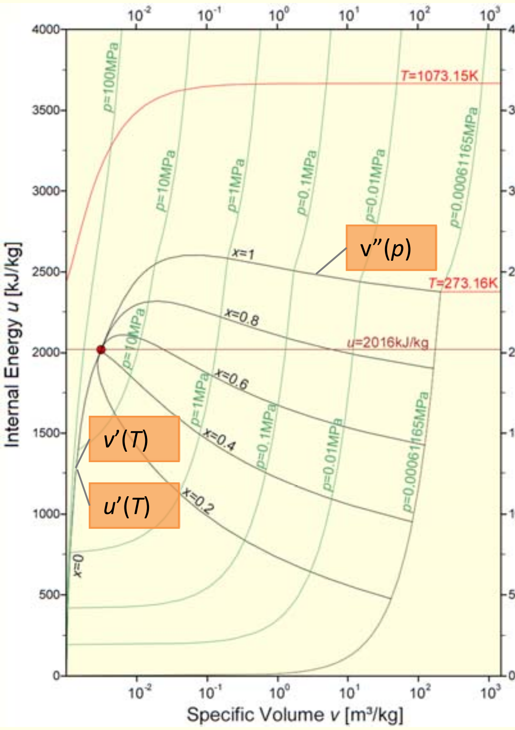
CTR **≈ 260 (590)**

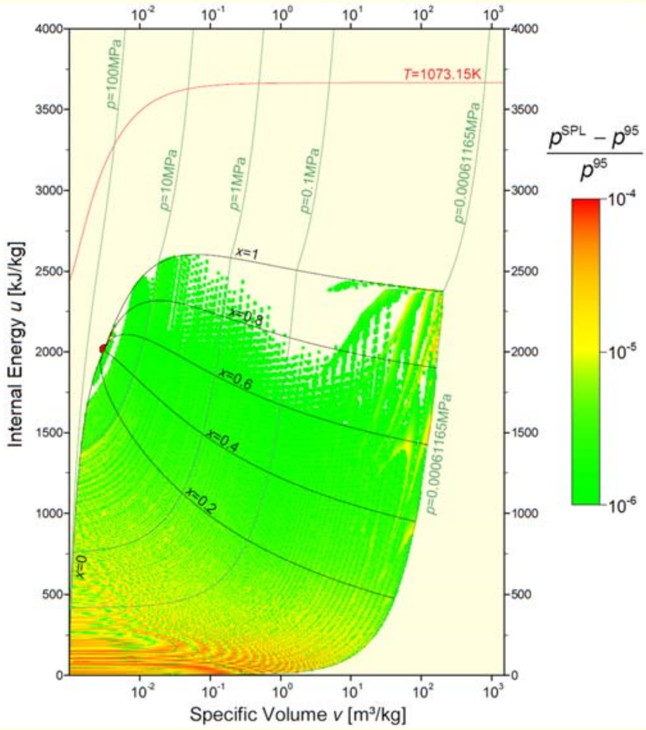
CTR **≈ 19 (160)**

Property Calculations for Water and Steam in CFD-Simulations

→ **Auxiliary Functions for Two-Phase Region:**

→ **Saturation Pressure $p_s(u,v)$:**





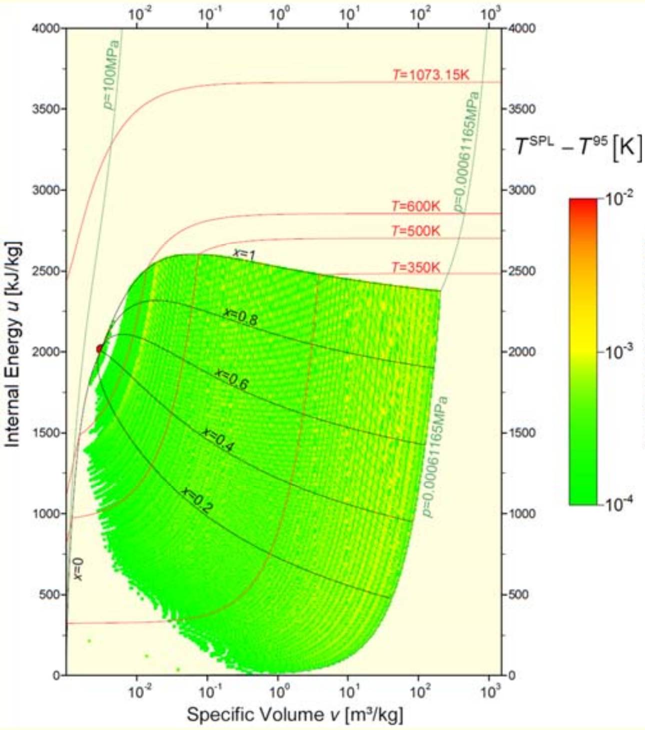
- High numerical consistency at dew curve
- Distinct phase test

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

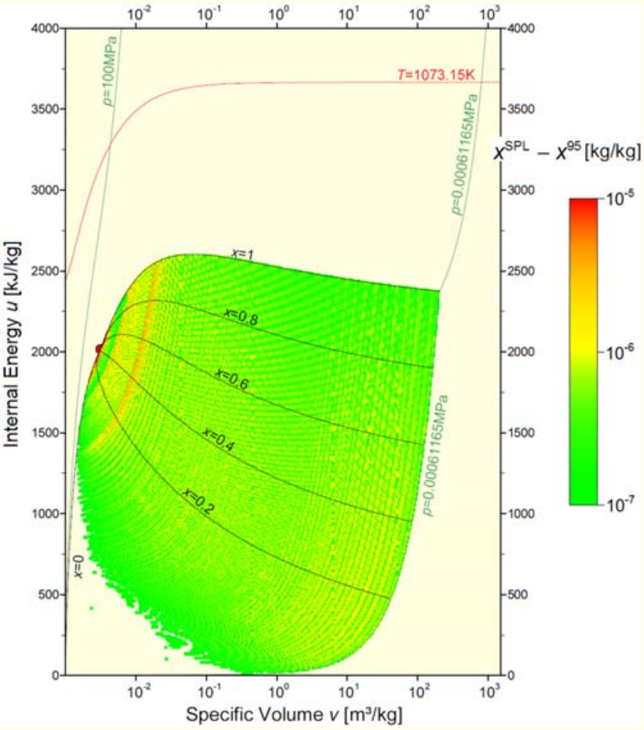
CTR **≈ 3 (490)**

Property Calculations for Water and Steam in CFD-Simulations

→ **Saturation Temperature $T_s(u,v)$:**



→ **Vapor Fraction $x(u,v)$:**

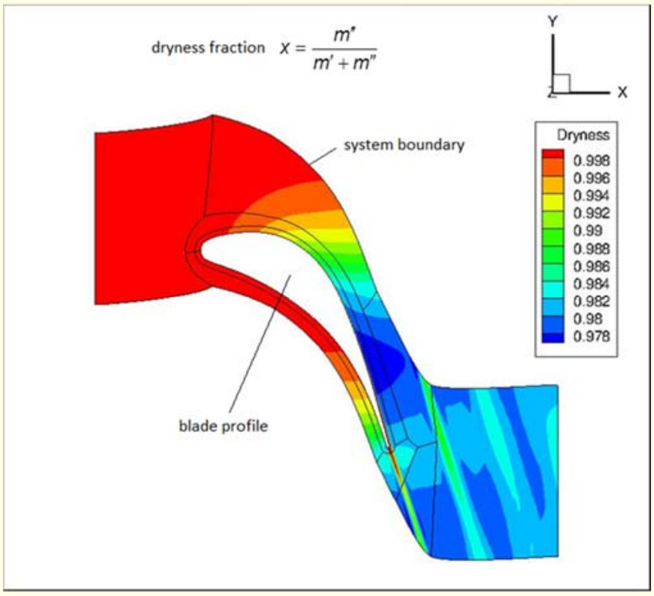


Computing time ratio in comparison to IAPWS-IF97 (IAPWS-95):

***CTR* ≈ 3 (490)**

Application of the Spline based Table Look-up Method in CFD

Steam flow at a fixed blade in a steam turbine (considering condensation):



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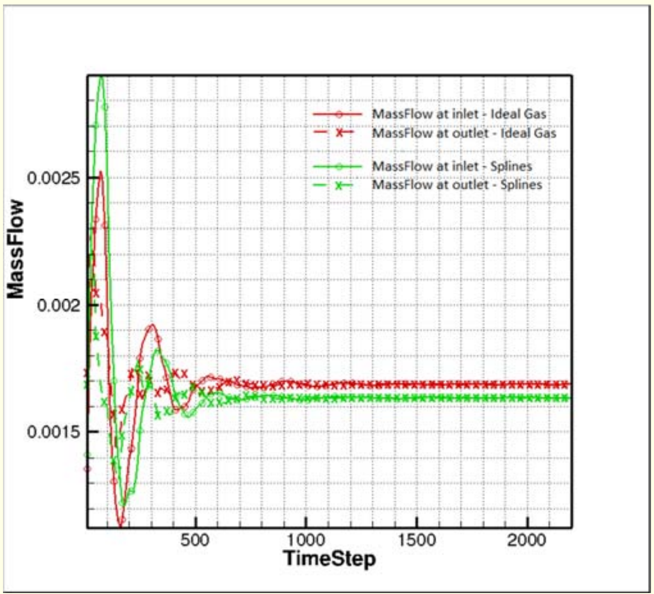
CFD-Software TRACE (DLR)

- **Application of spline-based property functions based on IAPWS-95**
- **14040 cells**
- **Hardware: 8 CPUs**

Application of the Spline based Table Look-up Method in CFD

Convergence: CFL-Factor (Courant–Friedrichs–Lewy-Factor)=30



- **Calculation with Spline 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**

The consideration of real fluid behavior with spline-based property functions requires only 40% additional computing time in comparison to a calculation with the ideal gas model.

Practical calculations:

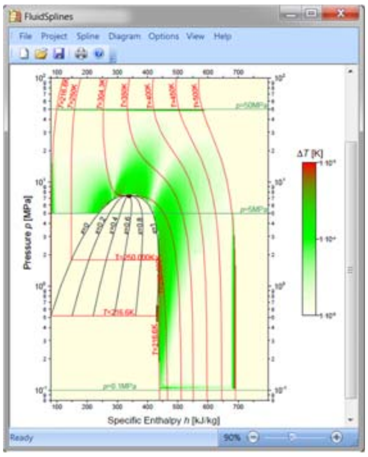
- **stage groups in 3D**
- **non-stationary process**

Computing time: several days

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

- **Spline-Based Table Look-Up Method:**
  - **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 ppm - the results of a process simulation will not change**
  - **Computing speeds can be increased by factors > 100 in comparison to the calculation from equations of state**
  - **Complete numerical consistency of forward and backward functions is possible**
- **Applicability in Computational Fluid Dynamics (CFD) has been demonstrated**
  - **Requirements of CFD and the calculation of non-stationary processes are fulfilled**
- **Software tool FluidSplines:**
  - **Application of the Spline-Based Table Look-Up Method to any fluid or function**
  - **Generation of spline-based property functions according to the requirements of a certain process simulation (range of validity, accuracy)**

⇨ **Proposal of a new guideline of International Association of Water and Steam (IAPWS):**

"IAPWS Guideline on the Fast Calculation of Steam and Water Properties in Computational Fluid Dynamics Using Spline Interpolation"

Thank you for your attention.