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# The 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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Francisco Blangetti, Alstom Power
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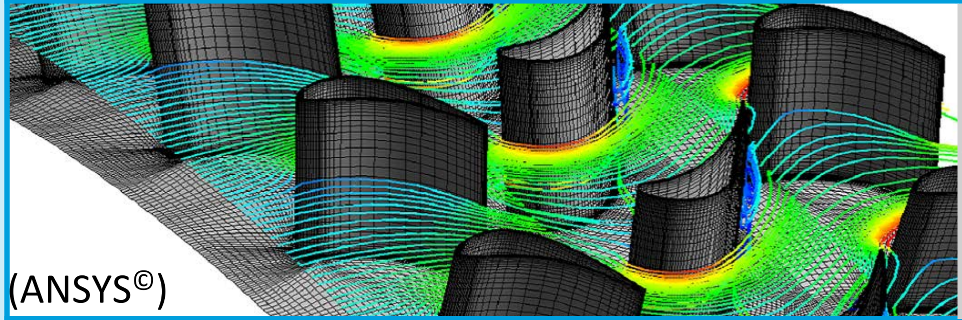
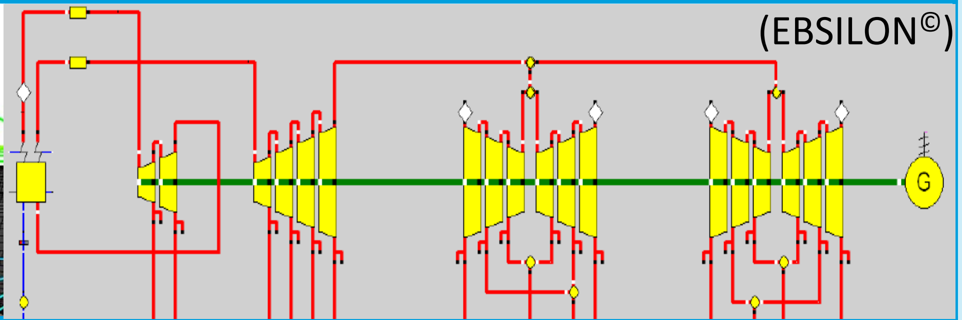
17th ICPWS, Prague (CZ), 2 – 6 September 2018

# Requirements for Property Calculation Algorithms in Extensive Process Simulations

| Computational Fluid Dynamics (CFD) | Heat Cycle Calculations (HCC) |
| --- | --- |
|  |  |





## Accuracy:

Deviations in calculated fluid properties lead to inaccurate mass, energy, and entropy balances.

⇨ **Property functions need to be very accurate!**

## Computing times:

Property functions are called extremely often, which consumes a large share of the overall computing time.

⇨ **Property functions need to be very fast!**

## Numerical Consistency / Differentiability:

Numerical solvers require continuity and numerical consistency of the equations to be solved.

⇨ **Property functions need to be numerically consistent and continuous differentiable!**

# Available IAPWS-Formulations for Water and Steam – Multi-parameter Equations of State

## Computing times:

Computing Time Ratio: $CTR = \dfrac{\text{Computing time of calculation from Peng-Robinson EOS}}{\text{Computing time of calculation from considered EOS}}$

$ANI$ = Average number of iterations

| *p*(*v*,*u*) | | | | |
|---|---|---|---|---|
| | **IF97 region 1** (liquid) | | **IF97 region 2** (vapor) | |
| **EOS** | *ANI* | ***CTR*** | *ANI* | ***CTR*** |
| Ideal gas | - | - | 3.83 | 1.47 |
| PR - EOS | 3 | 1.00 | 3.08 | 1.00 |
| IAPWS-IF97 | 2.94 | 1/6.08 | 3.64 | 1/11.1 |
| IAPWS-95 | 2.94 | 1/89.6 | 3.68 | 1/107 |

(Assumption: phase is known)

⇨ **Multi-parameter equations of state are too slow for CFD simulations!**

Convergence criteria:

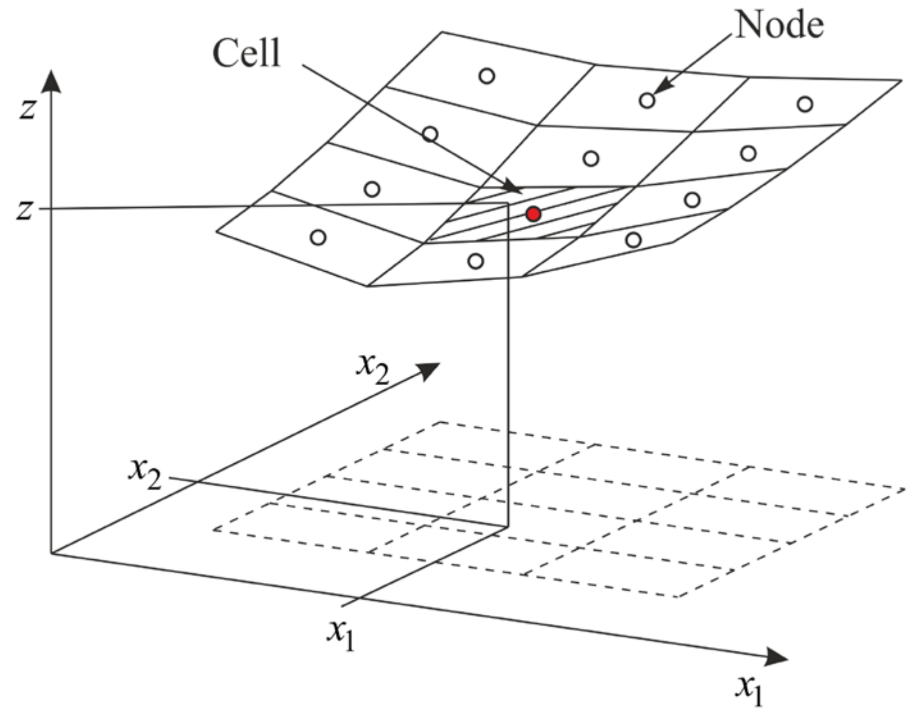
$$\left|\frac{\Delta v}{v}\right| \le 10^{-6}$$

$u \le 1\,\text{kJ/kg}$: $\quad |\Delta u| \le 10^{-6}\,\text{kJ/kg}$

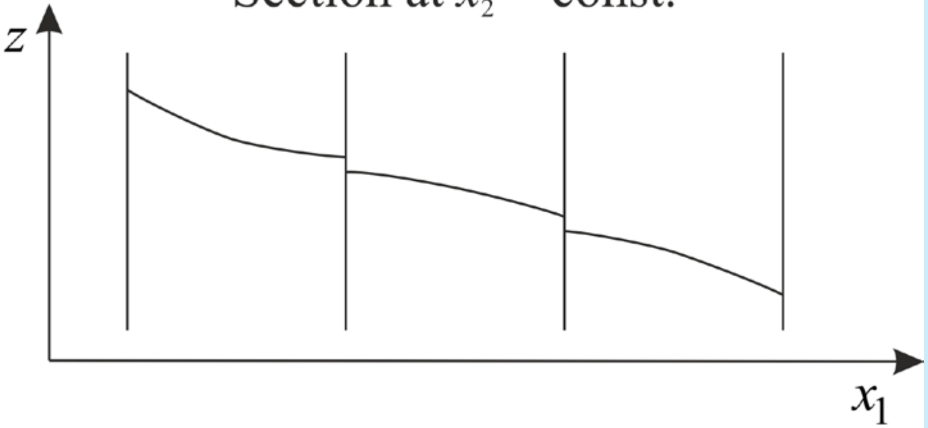
$u > 1\,\text{kJ/kg}$: $\quad \left|\frac{\Delta u}{u}\right| \le 10^{-6}$

# Available IAPWS-Formulations for Water and Steam – Table Look-up Methods

## Interpolation of any property function $z(x_1,x_2)$:




Section at $x_2$ = const.




- Tabulation of the desired fluid properties in a grid of nodes, where the values are calculated from a reference eq. of state.
- Calculation during process simulation:
  - Cell-search in the grid of nodes
  - Interpolation of $z(x_1,x_2)$:
    - local methods, for example:
      - bi-linear ($C^0$-continuous), z.B. ANSYS-CFX
      - TTSE (Taylor series expansion - discontinuous)

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

$$z_{\{i,j\}}(x_1,x_2)=z_{i,j}+\Delta x_{1,i}\left(\frac{\partial z}{\partial x_1}\right)_{x_2}+\frac{\Delta x_{1,i}{}^2}{2}\left(\frac{\partial^2 z}{\partial x_1{}^2}\right)_{x_2}+\Delta x_{2,j}\left(\frac{\partial z}{\partial x_2}\right)_{x_1}+\frac{\Delta x_{2,j}{}^2}{2}\left(\frac{\partial^2 z}{\partial x_2{}^2}\right)_{x_1}+\Delta x_{1,i}\Delta x_{2,j}\left(\frac{\partial z}{\partial x_1\partial x_2}\right)$$

# Available IAPWS-Formulations for Water and Steam – Table Look-up Methods

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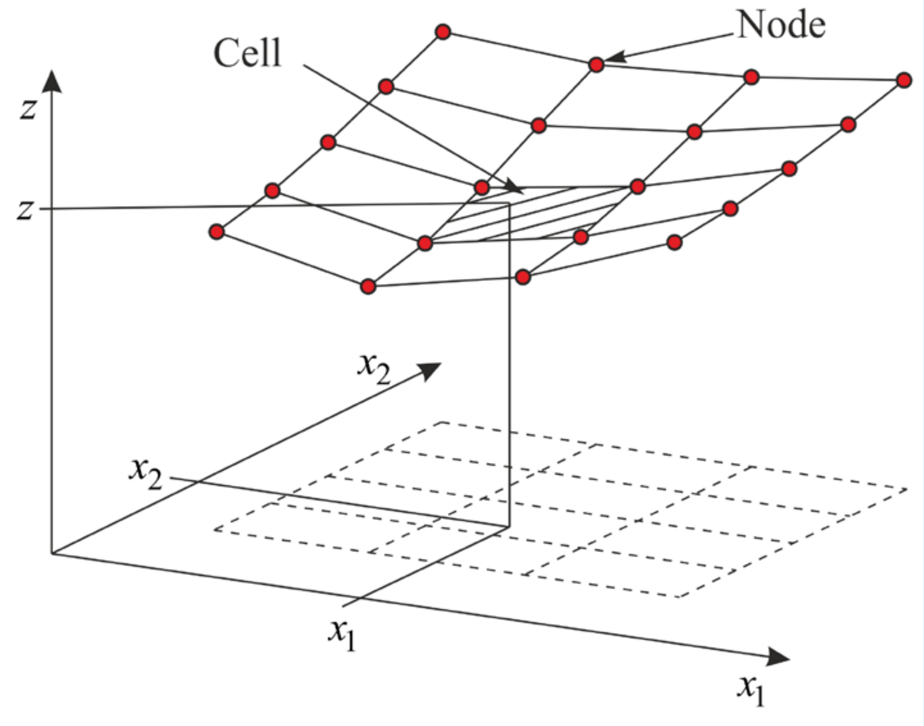


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    - – local methods, for example:
      - bi-linear ($C^0$-continuous), z.B. ANSYS-CFX
      - TTSE (Taylor series expansion - discontinuous)
    - – global methods, for example: bi-cubic spline function ($C^2$-continuous).

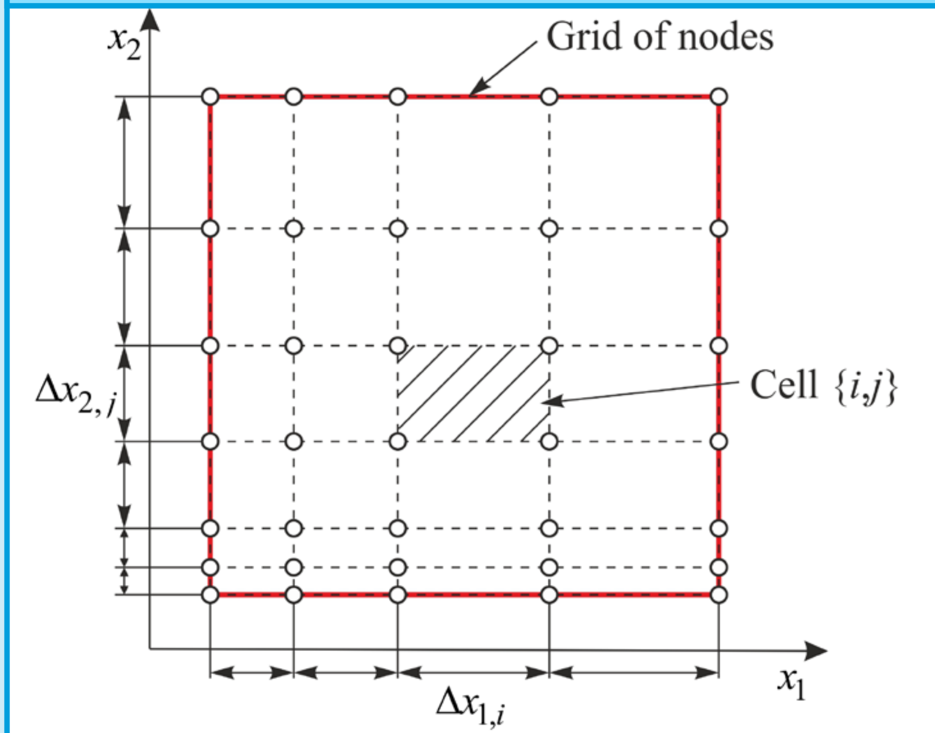
⇨ **Accuracy can be controlled with the number of nodes in the grid.**

⇨ **Computing times are mostly determined by the cell-search algorithm.**

⇨ **Look-up tables can easily be established using an existing equations of state.**
**→ Table look-up methods are very flexible!**

# Available IAPWS-Formulations for Water and Steam – Table Look-up Methods

## Interpolation of any property function $z(x_1,x_2)$:




- Tabulation of the desired fluid properties in a grid of nodes, where the values are calculated from a reference eq. of state.
- Calculation during process simulation:
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    - local methods, for example:
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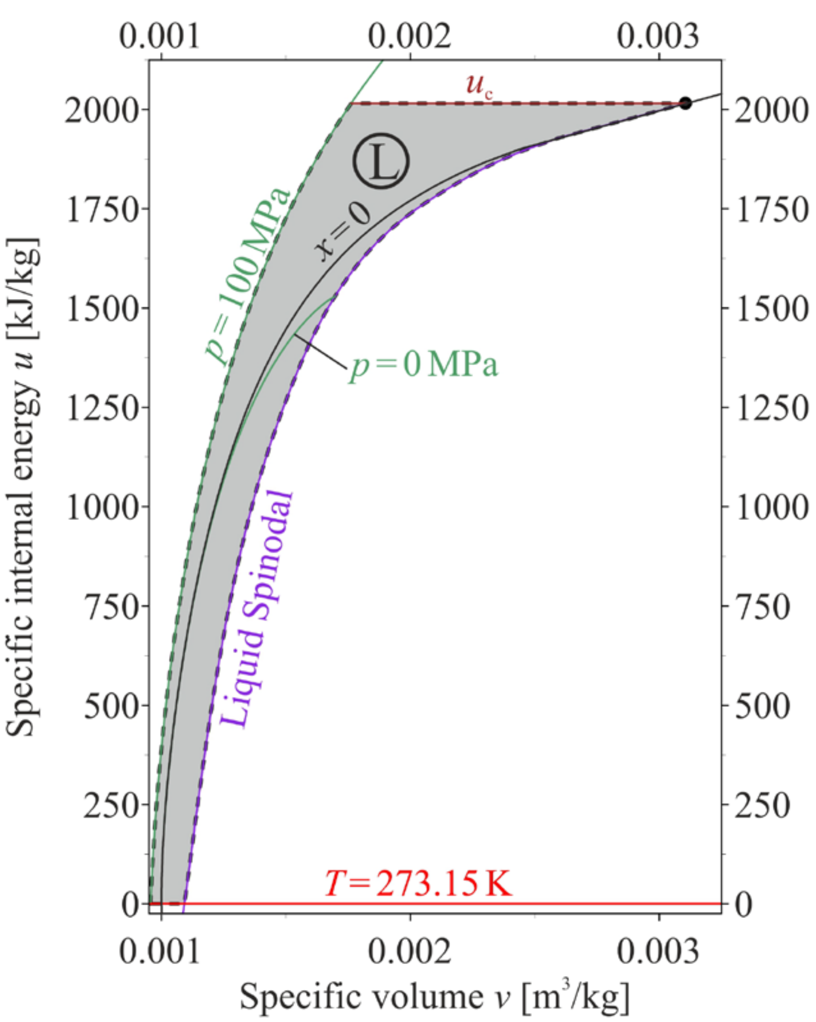
      - TTSE (Taylor series expansion - discontinuous)
    - global methods, for example: bi-cubic spline function ($C^2$-continuous).

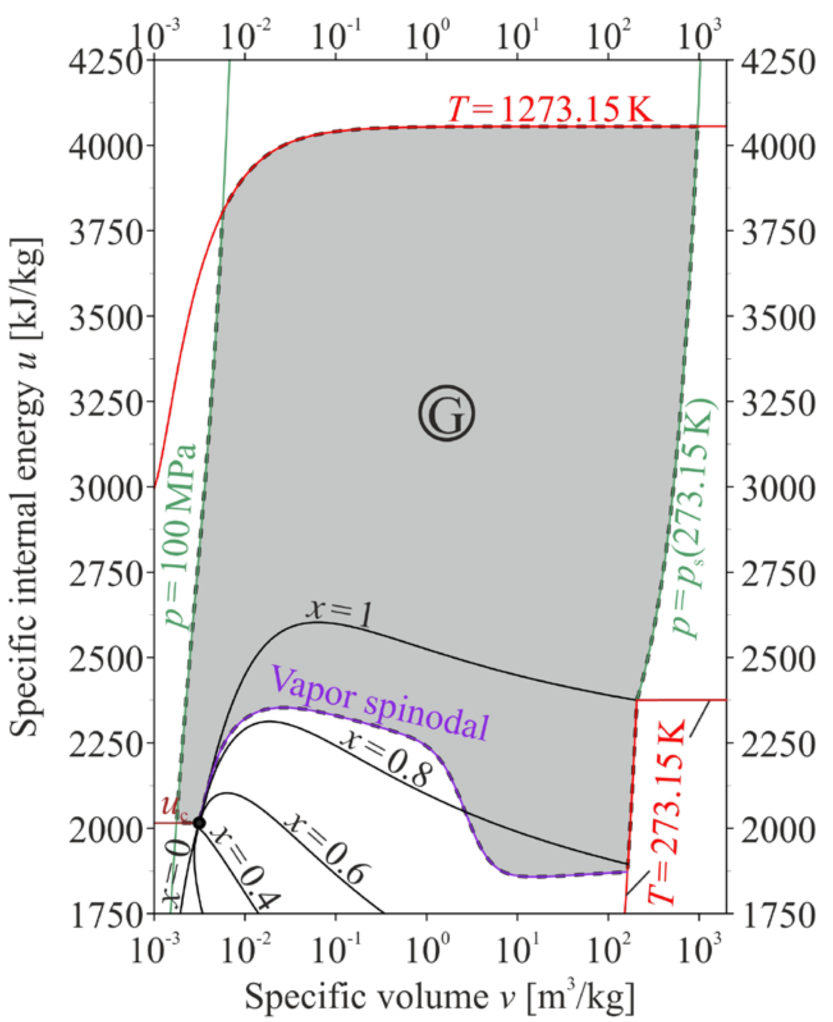
**Frequent problems:**

- To take the non-linearity of the property function into account, the node density varies across the grid (non-equidistant nodes) → extensive cell-search (computing times ↑)
- Polynomials of third or higher order → computationally intensive inverse functions
- Global methods require a grid of nodes with a rectangular outer boundary → unfavorable approaches to describe non-rectangular domains are often in use

# The Spline-Based Table Look-up Method (SBTL)

## Generation of a Spline-Function $p^{SPL}(v,u)$ based on the IAPWS-95:



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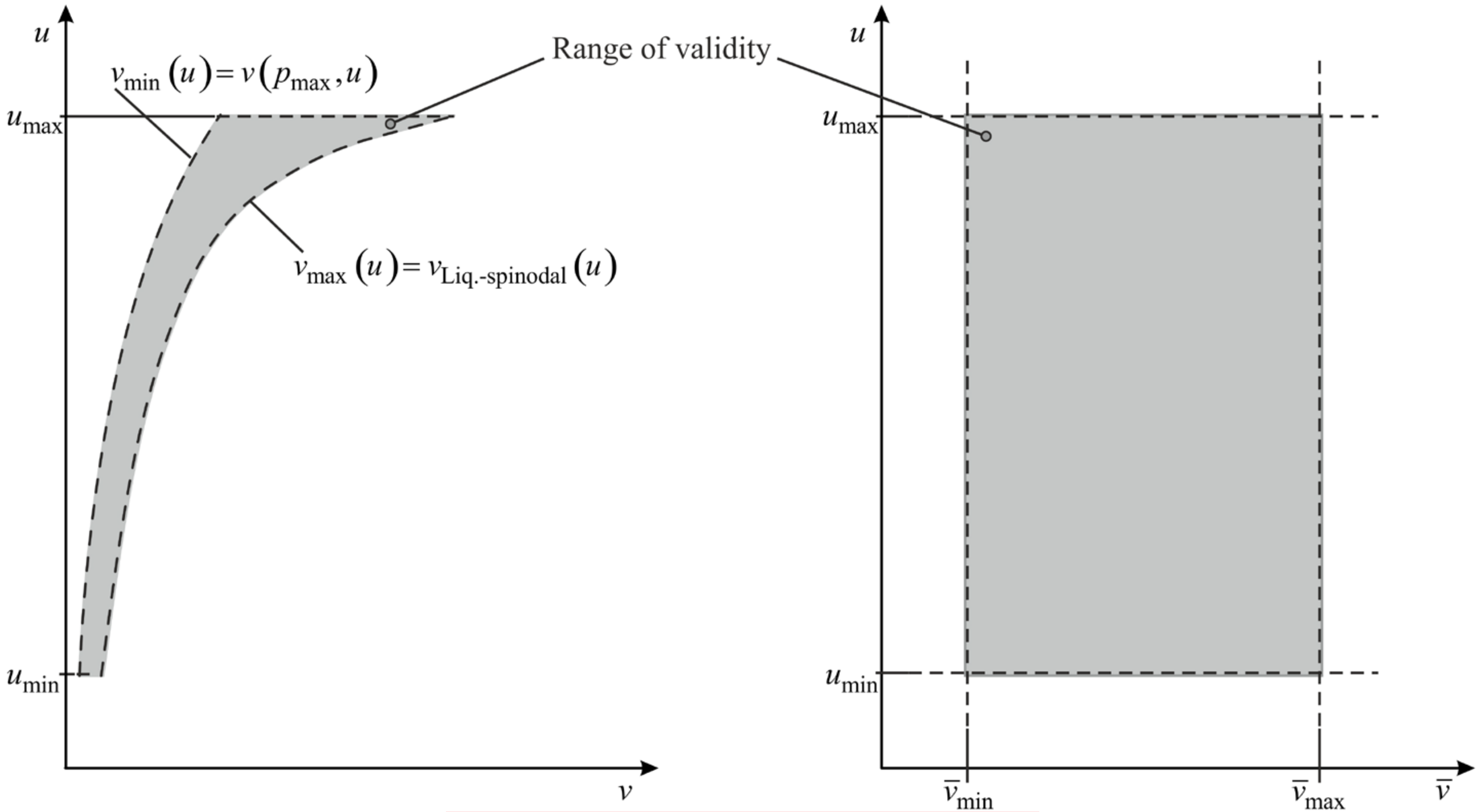


$$\overline{v}(v,u) = \frac{\overline{v}_{max} - \overline{v}_{min}}{v_{max}(u) - v_{min}(u)}\left(v - v_{min}(u)\right) + \overline{v}_{min}$$

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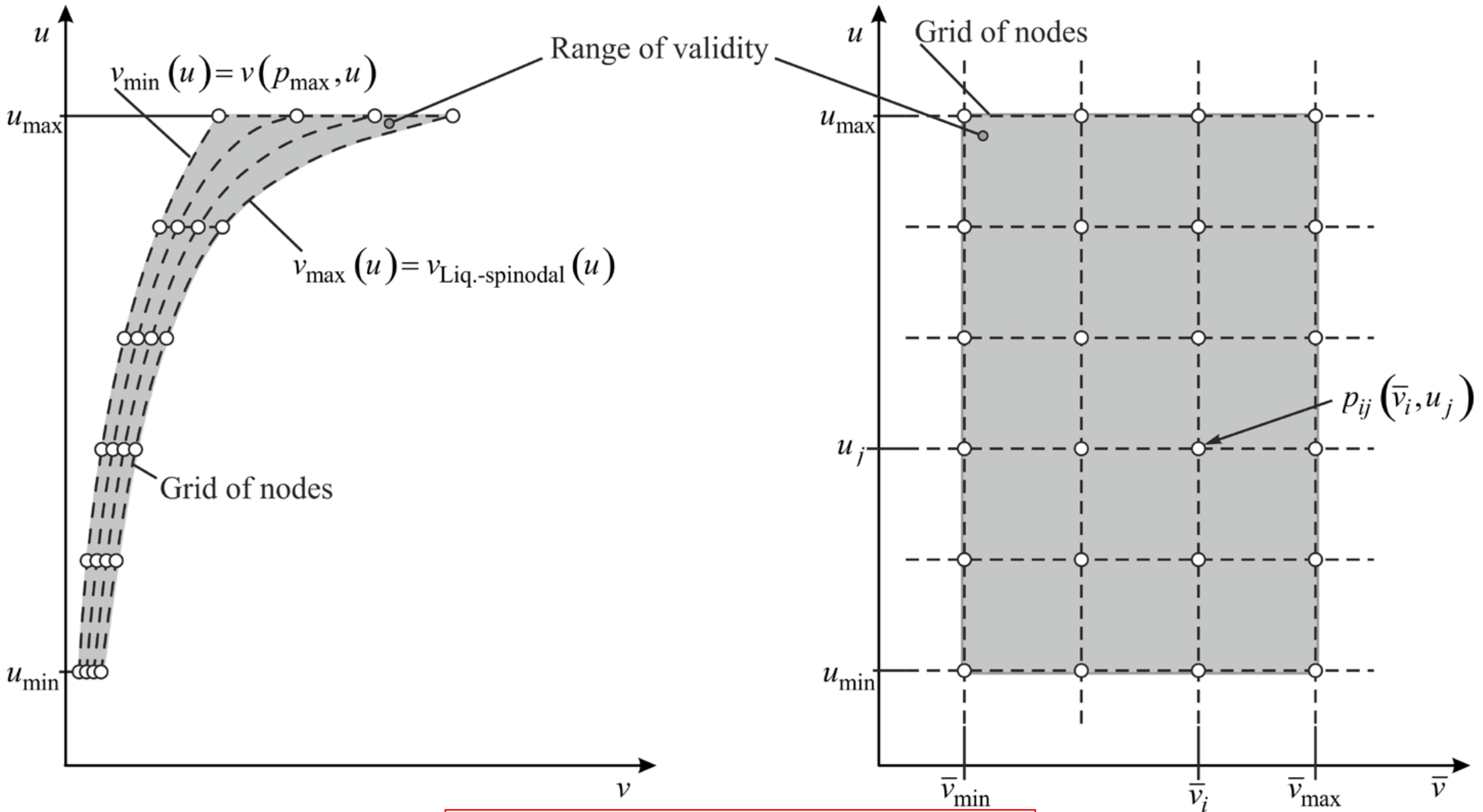
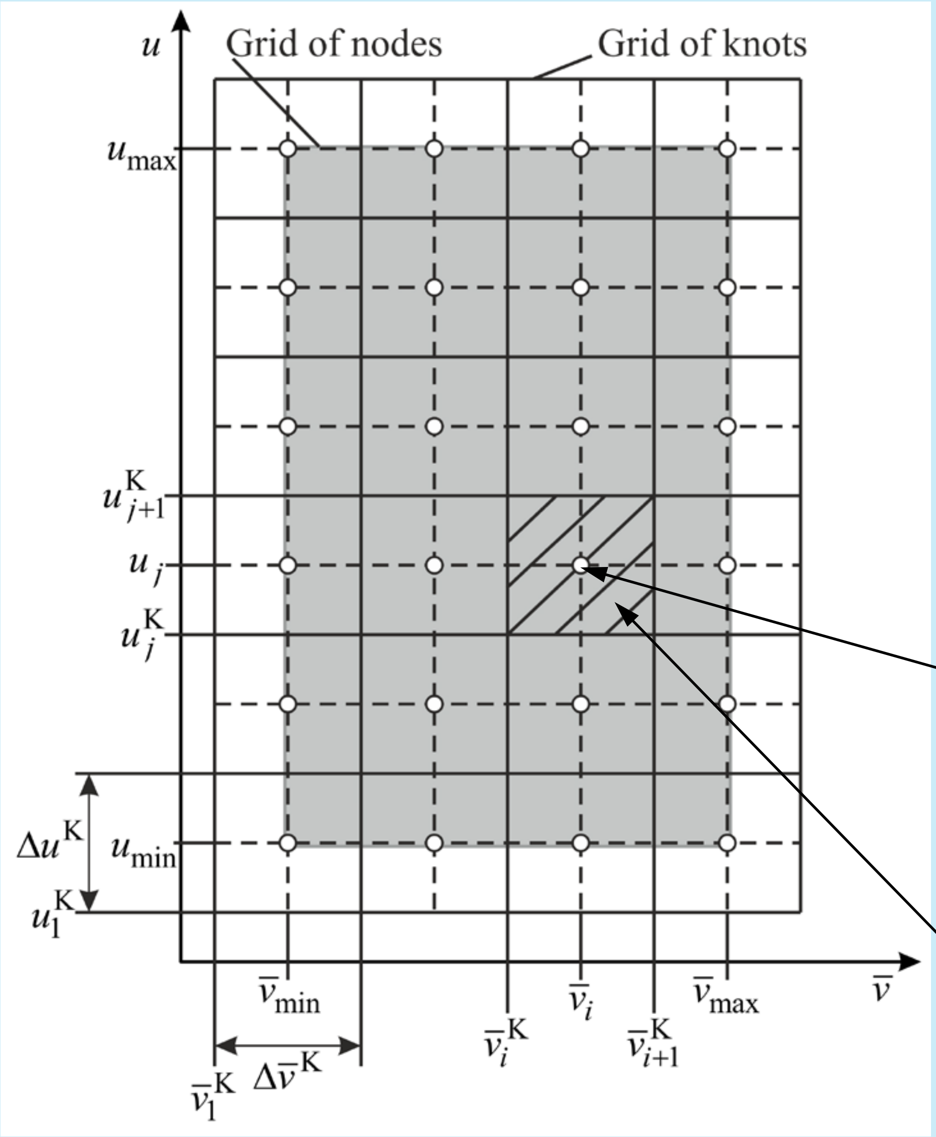



$$\bar{v}(v,u) = \frac{\bar{v}_{max} - \bar{v}_{min}}{v_{max}(u) - v_{min}(u)}\left(v - v_{min}(u)\right) + \bar{v}_{min}$$

# The **S**pline-**B**ased **T**able **L**ook-up Method (SBTL)

## Generation of a Spline-Function $p^{SPL}(v,u)$ based on the IAPWS-95:




- **Variable transformations ($v \rightarrow \bar{v}$):**
  - Transformation of an irregularly shaped domain into a rectangle
  - Linearization
    → Accuracy enhancement
- **Generation of a rectangular grid of nodes:**
  - $I$ nodes along $\bar{v}$ and $J$ nodes along $u$ (preferably equidistant for simplified cell search)
  - Calculation of node values

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

    from the underlying equation of state $p^{EOS}(v,u)$
- **Cell-definition in the grid of knots:**
  - Spline polynomial:

    $$p^{SPL}_{\{i,j\}}\left(\bar{v}, u\right) = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ijkl}\left(\bar{v} - \bar{v}_i\right)^{k-1}\left(u - u_j\right)^{l-1}$$

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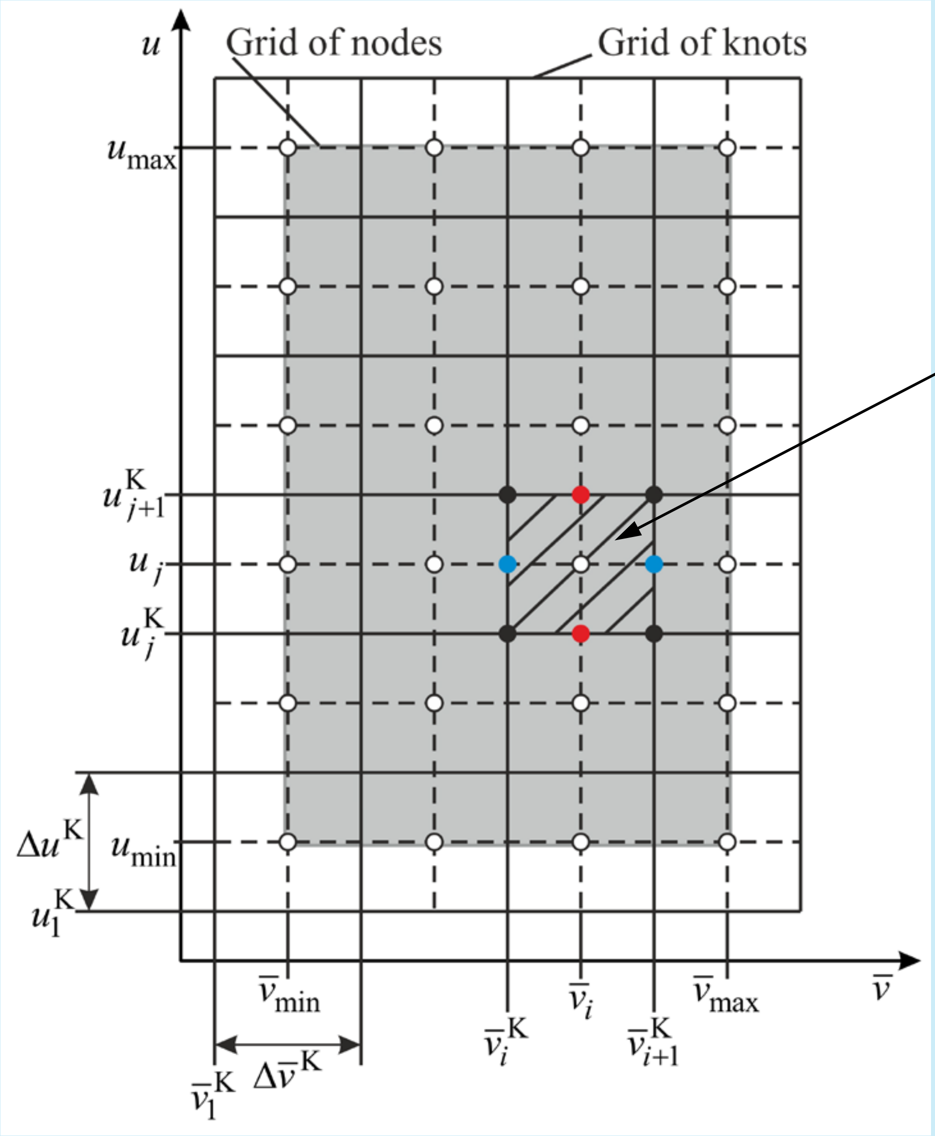


- **Variable transformations ($v \rightarrow \bar{v}$)**
- **Generation of a rectangular grid of nodes**
- **Cell-definition in the grid of knots:**
  - Spline polynomial:

$$p^{SPL}_{\{i,j\}}(\bar{v},u) = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ijkl}\left(\bar{v}-\bar{v}_i\right)^{k-1}\left(u-u_j\right)^{l-1}$$

- **Calculation of all $9IJ$ spline coeff. $a_{ijkl}$ from:**
  - $IJ$ interpolation conditions:

○ $p^{SPL}_{\{i,j\}}(\bar{v}_i,u_j) = p_{i,j}(\bar{v}_i,u_j)$

  - $3IJ+2(I+J)+1$ unknown derivatives:

● (blue) $(\partial p/\partial \bar{v})_u$ ● (red) $(\partial p/\partial u)_{\bar{v}}$ ● (black) $(\partial^2 p/(\partial \bar{v}\partial u))$

# The Spline-Based Table Look-up Method (SBTL)

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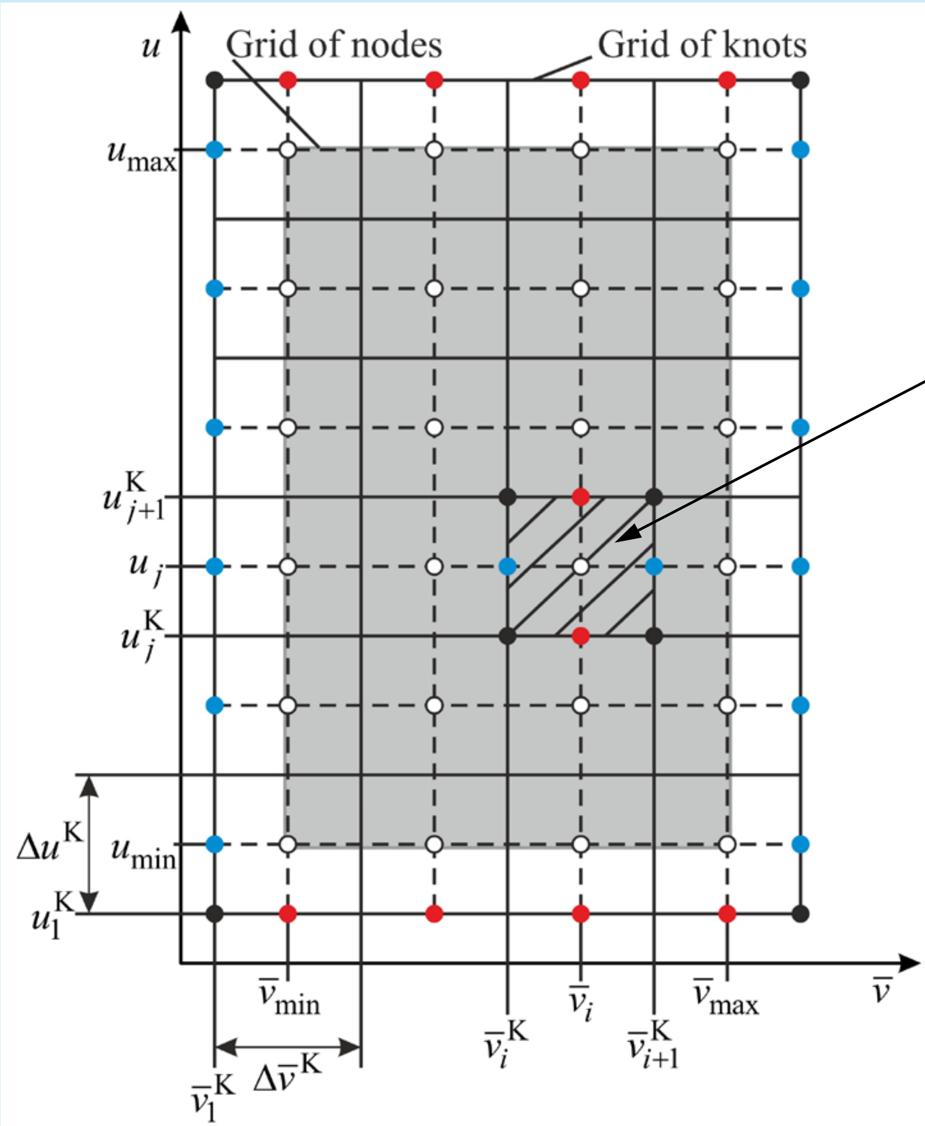


- **Variable transformations ($v \rightarrow \bar{v}$)**
- **Generation of a rectangular grid of nodes**
- **Cell-definition in the grid of knots:**
  - Spline polynomial:

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

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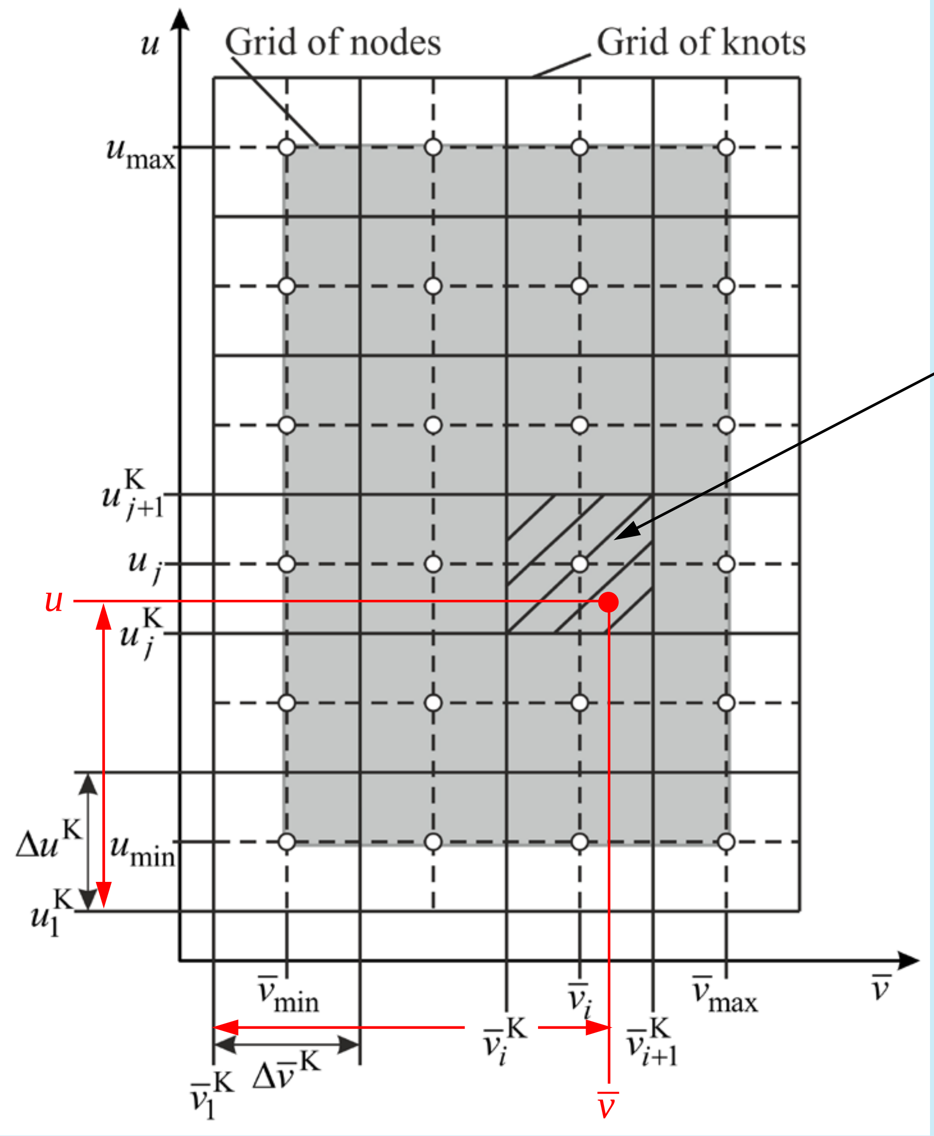
● (blue) $(\partial p/\partial \bar{v})_u$ ● (red) $(\partial p/\partial u)_{\bar{v}}$ ● (black) $(\partial^2 p/(\partial \bar{v}\partial u))$

When these $2(I+J)+4$ derivatives are given at the outer boundary of the grid of knots, the remaining unknowns can be obtained from $3(IJ-1)$ equations, so that the resulting spline function is continuously differentiable once.

# The Spline-Based Table Look-up Method (SBTL)

## Generation of a Spline-Function $p^{SPL}(v,u)$ based on the IAPWS-95:




- **Variable transformations ($v \rightarrow \bar{v}$)**
- **Generation of a rectangular grid of nodes**
- **Cell-definition in the grid of knots:**
  - Spline polynomial:

$$p^{SPL}_{\{i,j\}}(\bar{v},u) = \sum_{k=1}^{3}\sum_{l=1}^{3} a_{ijkl}\left(\bar{v}-\bar{v}_i\right)^{k-1}\left(u-u_j\right)^{l-1}$$

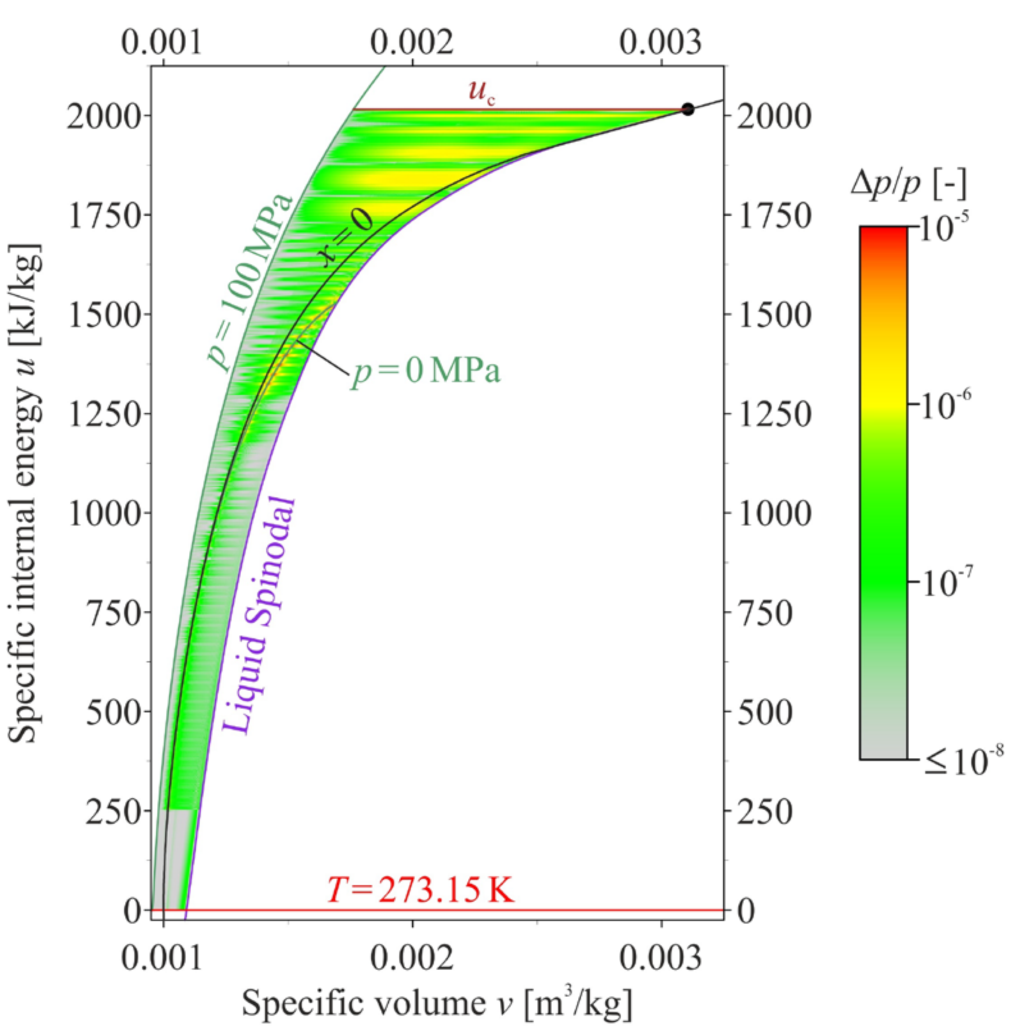
- **Calculation of all $9IJ$ spline coeff. $a_{ijkl}$:**
- **Grid optimization:**
  - for the desired accuracy
  - for minimal computing times
  - for minimal number of nodes (data)
- **Grid of knots along with all spline coeff. is stored for property calculations**
- **Evaluation of the SBTL property function:**
  - Transformation of $v \rightarrow \bar{v}$
  - Fast cell determination $\{i,j\}$:

$$i = \text{floor}\left(\frac{\bar{v}-\bar{v}^K_1}{\Delta\bar{v}^K}\right) \qquad j = \text{floor}\left(\frac{u-u^K_1}{\Delta u^K}\right)$$

  - Evaluation of the polynomial $p^{SPL}_{\{i,j\}}(\bar{v},u)$

# The Spline-Based Table Look-up Method (SBTL)

## SBTL function $p^{L}(v,u)$ – Deviations from IAPWS-95:




$$\overline{v}(v,u) = \frac{\overline{v}_{\max} - \overline{v}_{\min}}{v_{\text{liq.-spinodal}}(u) - v_{p\_\max}(u)} \left(v - v_{p\_\max}(u)\right) + \overline{v}_{\min}$$

**Grid of nodes:**

| $v$ [m³/kg] $\rightarrow$ $\overline{v}(v,u)$ | |
|---|---|
| **domain** | **grid lines** |
| $1 \leq \overline{v} \leq 20$ | 50 |
| $20 \leq \overline{v} \leq 40$ | 150 |
| $40 \leq \overline{v} \leq 95$ | 75 |
| $95 \leq \overline{v} \leq 100$ | 75 |

| $u$ [kJ/kg] | |
|---|---|
| **domain** | **grid lines** |
| $-8 \leq u \leq 250$ | 350 |
| $250 \leq u \leq 2040$ | 225 |

**Maximum deviations from IAPWS-95 in the stabile single-phase region:**

$p \leq 2.5$ MPa: $\quad \left|\Delta p / p\right|_{\max} = 0.092\ \%$

$p > 2.5$ MPa: $\quad \left|\Delta p\right|_{\max} = 2.74$ kPa

# The Spline-Based Table Look-up Method (SBTL)

## SBTL function $p^G(v,u)$ – Deviations from IAPWS-95:

**Grid of nodes:**

$v\ [m^3/kg] \rightarrow \bar{v}(v) = \ln(v)$

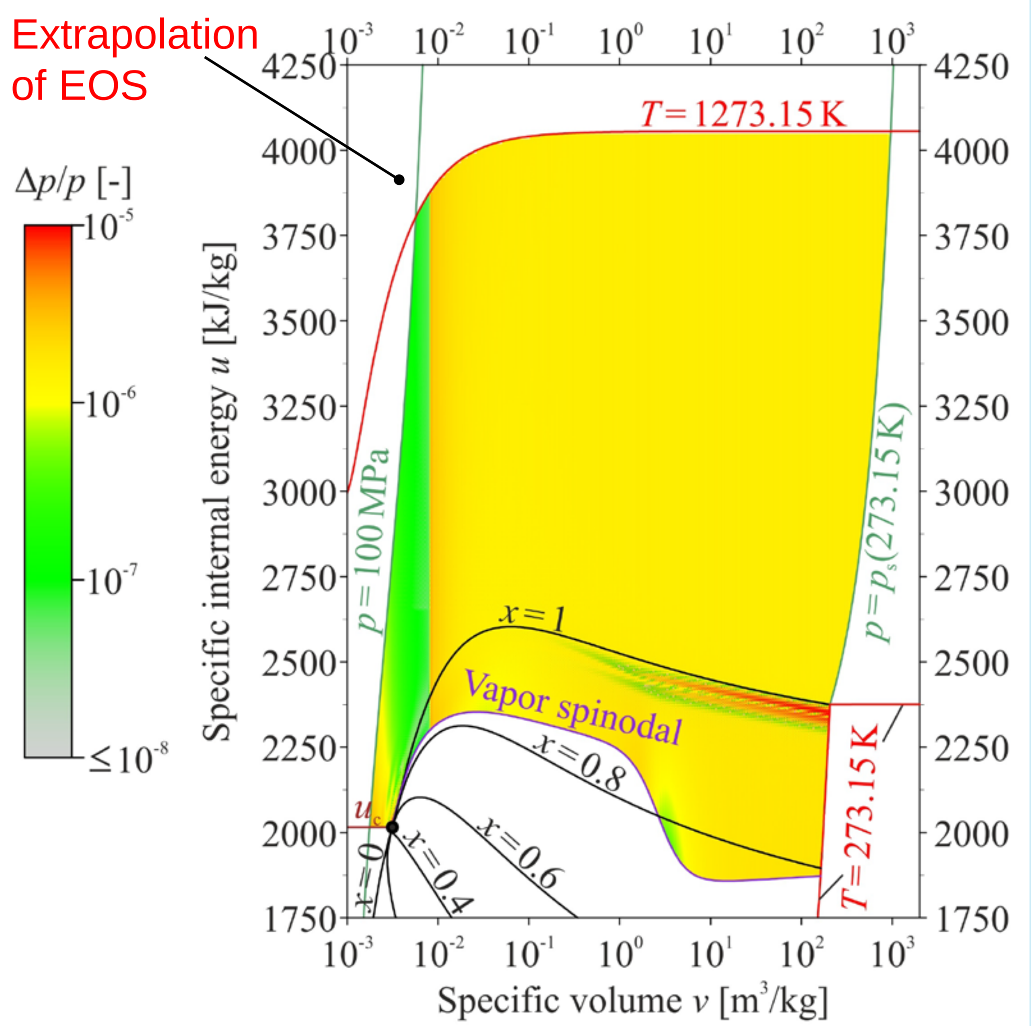
| domain | grid lines |
|---|---|
| $\bar{v}(1.6\times10^{-3}) \le \bar{v} \le \bar{v}(8\times10^{-3})$ | 100 |
| $\bar{v}(8\times10^{-3}) \le \bar{v} \le \bar{v}(1189)$ | 200 |

$u\ [kJ/kg]$

| domain | grid lines |
|---|---|
| $1845 \le u \le 2650$ | 100 |
| $2650 \le u \le 4085$ | 100 |

**Maximum deviations from IAPWS-95 in the stabile single-phase region:**

$$|\Delta p / p|_{max} = 0.001\,\%$$




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

# The Spline-Based Table Look-up Method (SBTL)

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

Spline function:

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

Inverse spline function:

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

with

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

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

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

and

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

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

Auxiliary spline function for fast determination of cell {*i*,*j*} : $u_{\{i,j\}}^{\text{AUX}}\left(p,\bar{v}\right)$

⇨ **The inverse spline function *u*(*p*,*v*) is numerically consistent with *p*(*v*,*u*).**

⇨ **The inverse spline function does not require extensive iterative algorithms.**

# The Spline-Based Table Look-up Method (SBTL)

## Application of inverse spline functions:

| **Spline functions of (*v*,*u*):** | | **(*p*,*v*):** | **(*u*,*s*):** |
|---|---|---|---|
| Pressure | $p^{\mathrm{SPL}}(v,u)$ → | $u^{\mathrm{INV}}(p,v)$ | |
| Temperature | $T^{\mathrm{SPL}}(v,u)$ | $T^{\mathrm{SPL}}, s^{\mathrm{SPL}}, w^{\mathrm{SPL}}, \eta^{\mathrm{SPL}}, \lambda^{\mathrm{SPL}}(v,u^{\mathrm{INV}})$ | |
| Spec. Entropy | $s^{\mathrm{SPL}}(v,u)$ → | | $v^{\mathrm{INV}}(u,s)$ |
| Speed of sound | $w^{\mathrm{SPL}}(v,u)$ | | $p^{\mathrm{SPL}}, T^{\mathrm{SPL}}, w^{\mathrm{SPL}}, \eta^{\mathrm{SPL}}, \lambda^{\mathrm{SPL}}(v^{\mathrm{INV}},u)$ |
| Dynamic Viscosity | $\eta^{\mathrm{SPL}}(v,u)$ | | |
| Thermal conductivity | $\lambda^{\mathrm{SPL}}(v,u)$ | | |

⇨ **Property functions are numerically consistent with each other.**

⇨ **All thermodynamic and transport properties including derivatives and inverse functions are calculated without iterations.**

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

**Contents:**

- **Fundamentals of the SBTL method**
- **SBTL property functions based on IAPWS-IF97**
  - SBTL functions of (*v*,*u*) with inverse Functions of (*p*,*v*) and (*u*,*s*)
  - SBTL functions of (*p*,*h*) with inverse Functions of (*p*,*T*), (*p*,*s*) and (*h*,*s*)
  - SBTL functions for the gas phase including the metastable region
- **SBTL property functions based on IAPWS-95**
  - SBTL functions of (*v*,*u*)
  - SBTL functions of (*p*,*h*)
- **Results of the evaluation:**
  - Deviations from the underlying IAPWS formulations
  - Computing-Time Ratios with regard to the underlying IAPWS formulations
  - Application of the SBTL method in extensive process simulations:
    - Computational Fluid Dynamics (CFD)
    - Heat Cycle Calculations

# Deviations SBTL Property Functions from underlying IAPWS Formulations

## Permissible deviations:

| SBTL functions | Region | | | |
|---|---|---|---|---|
| | | liquid | vapor | two-phase |
| $p(v,u)$ | $p \leq 2.5$ MPa: | 0.6 % | 0.001 % | 0.0035 % |
| | $p > 2.5$ MPa: | 15 kPa | | |
| $T(v,u)$, $T(p,h)$ | | 1 mK | 1 mK | 1 mK |
| $v(p,h)$ | | 0.001 % | 0.001 % | 0.001 % |
| $s(v,u)$, $s(p,h)$ | | $10^{-6}$ kJ/(kg K) | $10^{-6}$ kJ/(kg K) | $10^{-6}$ kJ/(kg K) |
| $w(v,u)$, $w(p,h)$ | | 0.001 % | 0.001 % | - |
| $\eta(v,u)$, $\eta(p,h)$ | | 0.001 % | 0.001 % | - |

Deviations with regard to IAPWS-95 near the critical point:

$|p_{max}| < 0.01$ %, $|T_{max}| < 10$ mK, $|v_{max}| < 0.03$ %, $|w_{max}| < 5$ %

➢ **The deviations of the SBTL functions with regard to the current IAPWS formulations are within the permissible values!**

# SBTL functions of (*v*,*u*) and inverse functions of (*p*,*v*) and (*u*,*s*) – Computing times in comparison with IAPWS-IF97 and IAPWS-95

**Computing-Time Ratio** $CTR = \frac{\text{Computing time of the IAPWS-IF97 (BWE) function}}{\text{Computing time of the SBTL function}}$

| SBTL function | IAPWS-IF97 region | | | | |
|---|---|---|---|---|---|
| | **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 |
| $u(p,v)$ | 2.0 | 6.4 | 2.8 | 5.6 | 3.2 |
| $v(u,s)$ | 43.5 | 66.4 | 78.8 | 16.2 | 134 |
| $T(p,h)$ | 17.2 (2.9[a]) | 23.9 (4.7[a]) | 585 (3.0[a]) | 18.1 | 53.4 |
| $v(p,h)$ | 18.7 (3.8[a]) | 23.5 (6.1[a]) | 671 (5.1[a]) | 5.5 | 46.1 |

a) Backward equation with limited numerical consistency, e.g. $T(p,h)$ and $h(p,T)$

**IAPWS-IF97:** Extended Steam Tables Software (includes determination of IAPWS-IF97 regions)

**IAPWS-95:** REFPROP (internal, highly optimized functions (phase is known))

**Processor:** Intel Xeon – 3,2GHz

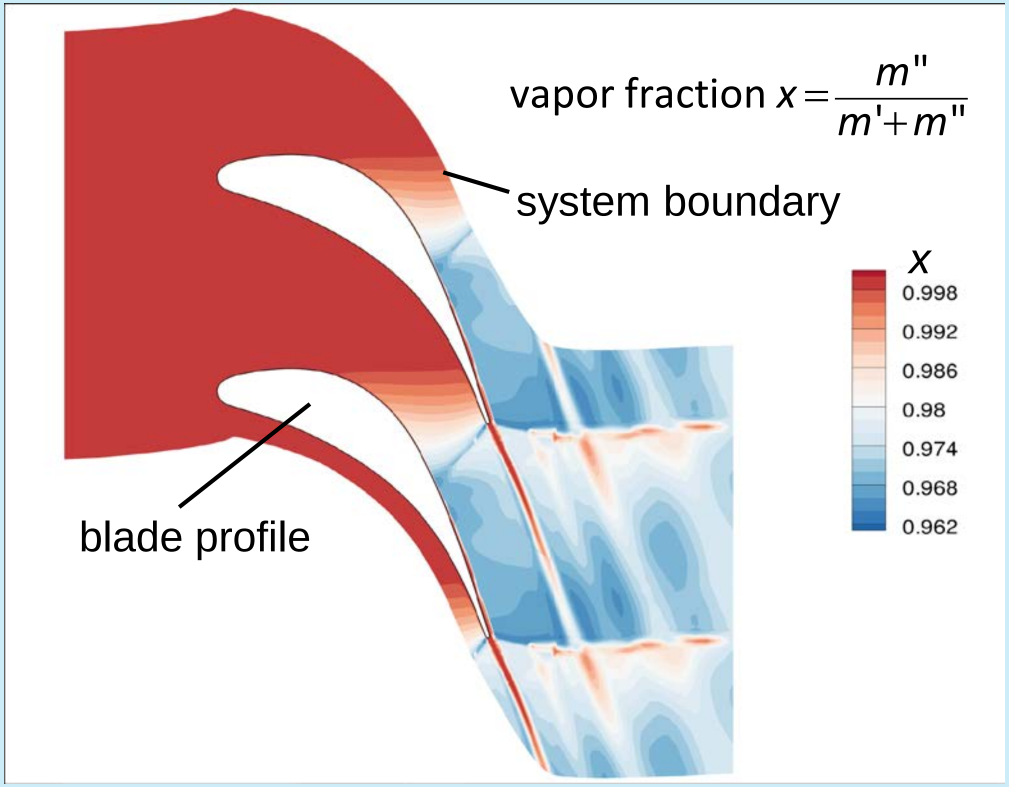
**OS:** Windows7 (32 Bit)

**Compiler:** Intel Composer XE 2011

➢ **SBTL functions are up to 270 (15000) times faster!**

# Application of the SBTL Method in Computational Fluid Dynamics (CFD)

## Simulation of 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)**

- **Implementation of SBTL property functions based on IAPWS-IF97**
- **Extensive assessment of simulation results, computing times, and convergence behavior**

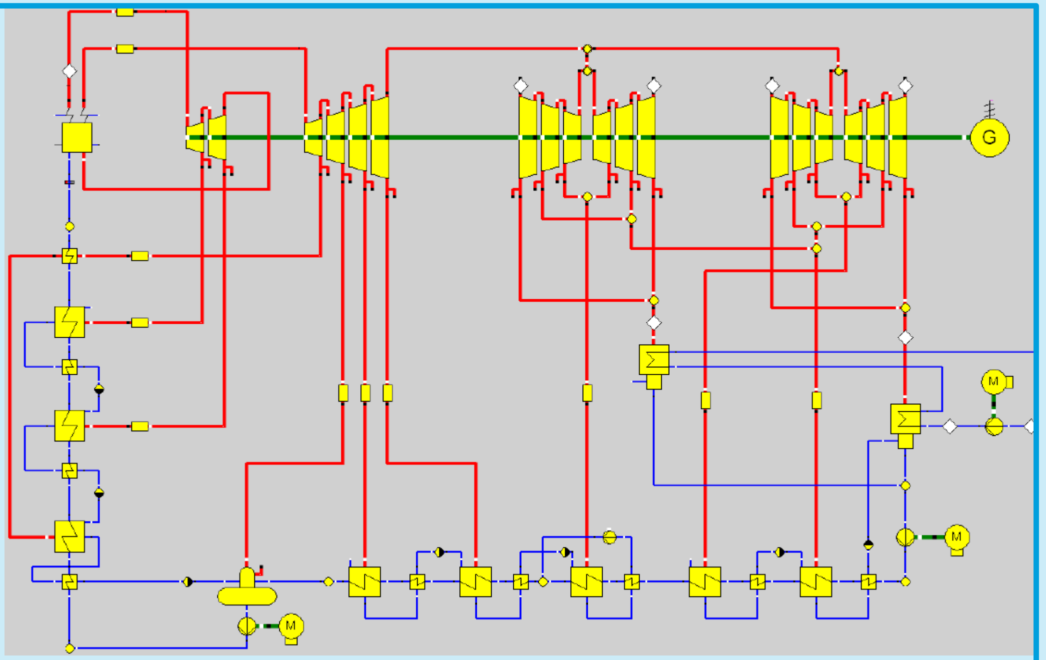
**Application of the SBTL method:**

- **in comparison with the direct application of IAPWS-IF97:**
  - **the computing times are reduced by factors of 6 - 10!**
  - **the differences in the results of the process simulations are negligible!**
- **in comparison with the application of the ideal gas-model:**
  - **the computing times are increased by a factor of 1.4 only!**

# Application of the SBTL Method in Heat Cycle Calculations

➢ **EBSILON Professional**
(STEAG Energy Services)

➢ **KRAWAL-modular**
(SIEMENS PG)




Implementation of SBTL property functions of (*p*,*h*) and the corresponding inverse functions of (*p*,*T*), (*p*,*s*), and (*h*,*s*) based on IAPWS-IF97:

⇨ **For a typical simulation of a conventional power plant in EBSILON Professional, the share of property calculations in the overall computing time is reduced from 25 % to 8 % and the overall computing time is reduced by 17 %.**

⇨ **In KRAWAL-modular, the overall computing times are reduced on average by 50 %.**

⇨ **The differences in the results of the process simulations are negligible (< 0.02 %).**

# Further Applications of the SBTL Method

- **Fluids:**
  - **Helium**
  - **Nitrogen**
  - **Carbon dioxide**
  - **Humid air**

- **Software:**
  - **RELAP-7** (Reactor Excursion and Leak Analysis Program), developed at the Idaho National Laboratory (INL), USA
  - **ATHLET** (Analysis of THermal-hydraulics of LEaks and Transients), developed at the GRS, Germany
  - **SubChanFlow** and **TwoPorFlow** (thermal-hydraulic codes), developed at KIT, Germany
  - **DYNAPLANT** (simulation of non-stationary processes in power plants), developed by SIEMENS, PG, Germany

# 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 270 times faster than IAPWS-IF97)
- **Method has been tested in extensive process simulations:**
  - in Computational Fluid Dynamics (CFD):
    - enables consideration of the real fluid behavior with high accuracy
    - 6-10 times faster than simulations with IAPWS-IF97
    - with regard to the ideal-gas model, the computing times increase by 40 % only
  - in Heat Cycle Calculations:
    - with regard to the direct application of IAPWS-IF97, the overall computing times are considerably reduced (17 % - 50 %)
    - the differences in the results of the process simulations are negligible

**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)**



President:
Dr. David Guzonas
Canadian Nuclear Laboratories
Chalk River, Ontario, Canada

- **Adopted at the IAPWS Annual Meeting in 2015 (Stockholm, Sweden)**

# Thank you for your attention!