





Accurate and Fast Calculation of Thermophysical Properties for Water and Steam in the ATHLET Code Using the Spline-Based Table Look-Up Method (SBTL)

Based on IAPWS-95

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#### **Outline**

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#### **Motivation**



- thermophysical properties of fluids an essential part of fluiddynamic simulation tools like AC<sup>2</sup>-codes
- general requirements
  - properties and their derivatives
  - wide range of validity
  - numerically consistent backward functions
  - at least one time continuously differentiable functions
  - → <u>accurate and fast</u> algorithms for calculation



## **Objective**



- fast and accurate library for fluid property of water and steam based on
  - scientific standard IAPWS-95
  - Spline-Based Table Look-Up Method (SBTL method)
- implementation into the ATHLET-code
- verification and validation

# **General aim**

Improvement of ATHLET-code regarding accuracy of results and computing time by implementation of new fluid properties library for water and steam



### Scientific Standard IAPWS-95



- International Association for the Properties of Water and Steam (IAPWS)
- "IAPWS Formulation 1995 for the Thermodynamic Properties of Ordinary Water Substance for General and Scientific Use" (IAPWS-95)
  - thermodynamic water and steam properties
  - fluid phases, incl. vapour-liquid equilibrium and metastable states
  - region: 273.15 K ... 1273 K and 611,212 Pa ... 1000 MPa
- additional releases for
  - viscosity, conductivity, surface tension



# Spline-Based Table Look-Up Method



### table look-up method:

 determination of values from previously tabulated data points by interpolation

### SBTL: combination of

- (bi-quadratic) polynomial spline interpolation techniques and
- specialized coordinate transformations

#### features

- high accuracy and low computing time
- SBTL property functions at least one time continuously differentiable
- inverse spline functions numerically consistent with corresponding forward spline functions



# Spline-Based Table Look-Up Method



# General approach

- generation of SBTL function
  - transformation of variables (mapping for higher accuracy)
  - generation of a grid (discrete data points / nodes)
  - grid optimization
  - calculation and storage of nodes and spline coefficients
- calculation of value with SBTL method
  - transformation of variables
  - determination of corresponding node in the grid
  - calculation of spline polynomial using stored spline coefficients
  - optional: inverse function or derivatives



# Spline-Based Table Look-Up Method



# Software library

- C++ library
- software realization of SBTL method
- implementation into the Fortran-code of ATHLET (function calls)
- platform independent (Windows, Linux)



## Concept



- determination of necessary thermophysical properties, transport properties and derivatives for ATHLET-code
- independent variables (ATHLET: pressure, temperature)
- development of the SBTL software library for fluid properties
- implementation of library into the ATHLET-code
- analysis of accuracy and computing time
- verification and validation of
  - software library and
  - ATHLET-code with new library for fluid properties



## **Summary and Outlook**



- implementation of <u>accurate and fast</u> calculation of thermophysical properties for water and steam into the ATHLET-code
- intensive verification and validation process
- further extension to other codes of system AC<sup>2</sup>
- extension to other fluids in ATHLET / AC<sup>2</sup>





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