Speed up of thermodynamic libraries usage through dynamic spline interpolation

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Plan of presentation

- Introduction – what is PSRE Co and PASS software
- PSRE Co and CO-LaN
- How to speed up interaction
  with thermodynamic libraries

About PSRE Co

- Founded in 1992 on the base of Piping Systems Lab VNIPIneft
- >30 years of CAD/CAE experience
- Developer of
  - CAE software for piping and equipment
  - International and Russian Technical standards and guides
- Member(s) of AIhE, DIERS, EDUG, TUFFP, CO-LaN, ASSESS Initiative
- Many years of cooperation with leading vendors of Plant Design CAD systems and leading CAPE software vendors
- **See our software now on www.passuite.com !**

CAE software from PSRE Co

Piping Analysis & Sizing Suite (PASS)

Process Engineering software (Heat exchange and fluid flow simulation)

Pressure
Relief systems
Analysis
(**Relief**)

Piping Flow Analysis
Pressure drop and
Heat losses
(**Hydrosystem**)

Piping
and Equipment
Thermal Insulation
Design and Analysis
(**Insulation**)

Piping and equipment Stress Analysis
(**START**, **PASSAT**, **Nozzle-FEM**)

PASS Heat Exchange and Fluid Flow Simulation (CAPE) software

Hydrosystem

[redacted]

[redacted]

Fluid composition

Insulation

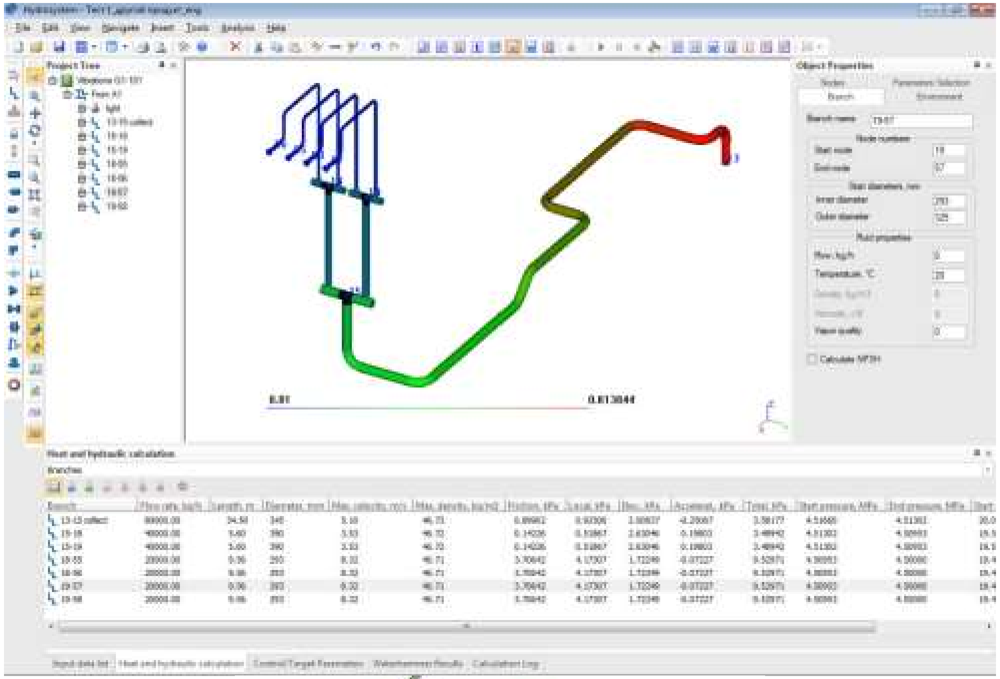
(Piping network)

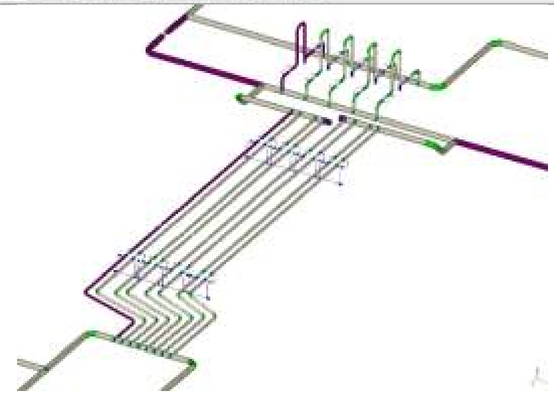
Shared libraries and databases

Climatology module	Thermodynamics STARS, WSP, Simulis, GERG Piping network analysis	Insulation and other materials
Soil properties	Report generator List & Label	Pipe materials

What is PASS/Hydrosystem software

- Piping network flow analysis commercial software
- Widely used for
  - process piping (hundreds of users)
  - out-doors gas, heat and water network
  - oil & gas field gathering systems
- **Powerful tool for everyday use for ANY process and piping engineer**

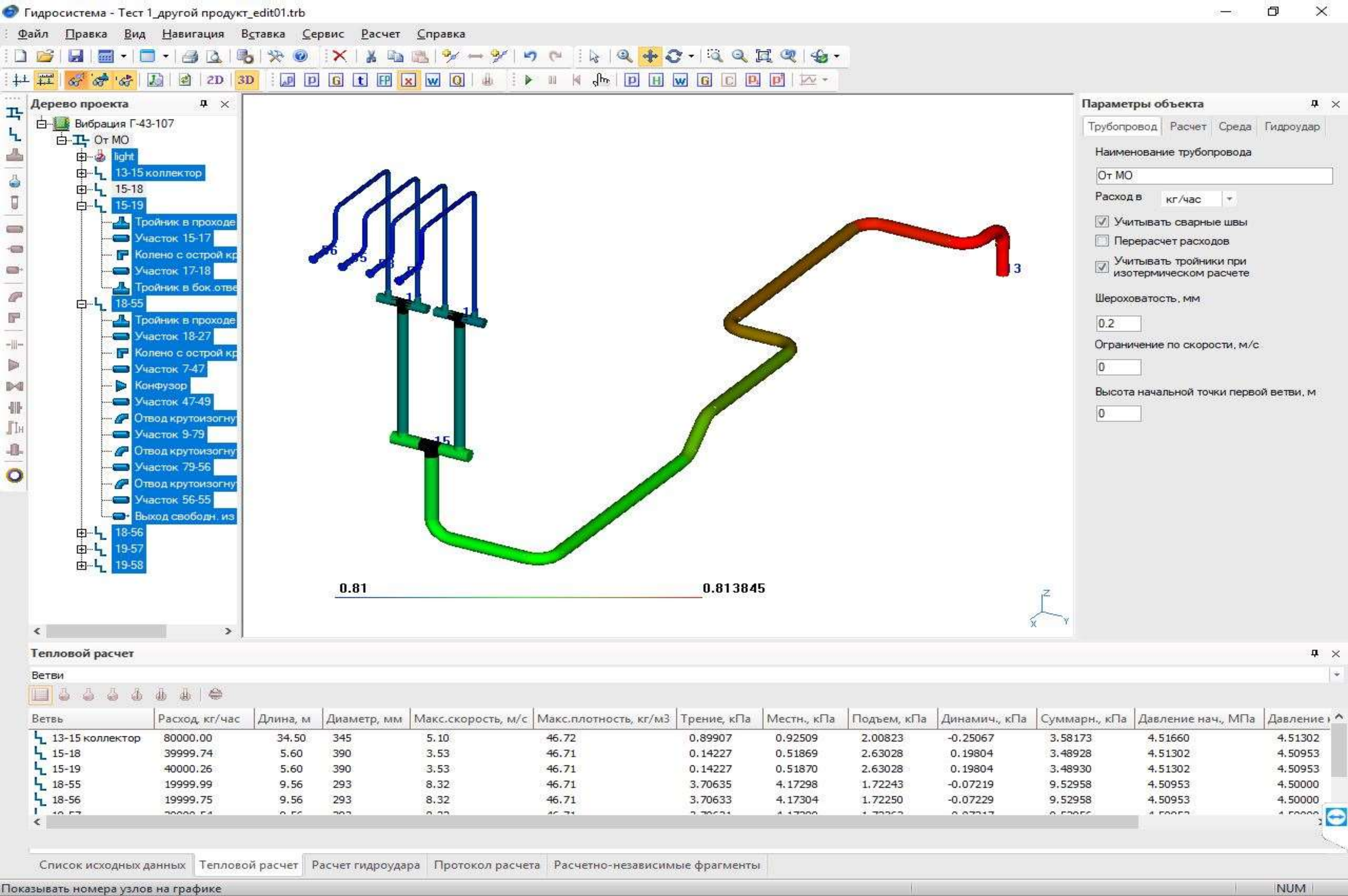




What is PASS/Hydrosystem software

- Steady state flow in complex piping networks
(flow distribution, pressure drops, heat losses)
  - Real liquids and gases
  - Multiphase Flow (Patterns)
    - Gas-liquid (with vaporization and condensation)
      - TUFFP Unified model
    - Gas-oil-water
    - Slurry flow
      - DHLLDV Framework Delft University model
    - Flow assurance
      - Severe slugging
      - Gas Hydrates precipitation
  - Choked flow
- Waterhammer
- Sizing and optimization
  - Diameters
  - Centrifugal pumps (Spaix)
  - Safety valves
  - Control valves
- Unbalanced forces calculation and export to piping stress analysis software
- 3D CAD import/Export

Flow distribution in complex piping networks



PSRE Co and CAPE OPEN

- Member of CO-LaN from 2011
- Long term business cooperation with several active members of CO-LaN
  - ProSim S.A.
  - Ruhr-Universität Bochum Chair of Thermodynamic (GERG-2008)
  - Tulsa University (TUFFP)
  - Chemstations
  - Linde Engineering
- Leading Hydrosystem developers (Elena Yudovina, Leonid Korelstein) passed CAPE-OPEN training in ProSim in 2013
- Active participants of Hydrodynamic SIG

PSRE Co and CAPE OPEN

- CAPE OPEN plans for PASS/HYDROSYSTEM
- PASS/HYDROSYSTEM as PME
  - Thermo Interface
  - Unit Interface
- PASS/HYDROSYSTEM as PMC
  - Unit Interface
- Plans were delayed because some part of goals were achieved by direct or specific COM integration and CAPE-OPEN interfaces looked complicated and time-consuming
  - Simulis Thermodynamics (ProSim)
  - GERG-2008 (Ruhr-Universität Bochum)
  - PVTSim Open Hydrate (Calsep)
  - Spaix for centrifugal pump sizing and selection (VSX)
- Now we are going to reconsider our plans and look at COBIA

PASS/HYDROSYSTEM and THERMO

- PASS/HYDROSYSTEM as PME calls different thermo PMCs for Phase Equilibruim (PE) and Thermophysical properties (TPP) of fluids in process of calculations
- Many iterations (embedded cycles) in PME => huge # of Thermo PMC calls
- The more complex is the case (like: “optimization of complex piping network with multiphase multicomponent fluid with heat exchange and multiple choked flow”), the more is the # of calls

- # of call is of orders from 10^4 to 10^6
- In complex calculation up to 90% software time is in Thermo PMC!
- We need to radically decrease # of Thermo PMCs calls!

Dynamic interpolation (table look up)

- PME needs to get PE and TPPs vs fluid parameters (p, T) or (p, h) or (p, s) in some region of parameters
- Let's evaluate this region and build reasonable grid with <u>not very big # of points </u>(up to 10^3)
- Preliminary calculate PE and TPPs in grid points
- Build interpolation for PE and TPPs using these data which would provide necessary accuracy and
  - Could be easily extended (rebuilt) if parameter region is extended
  - Rebuilt interpolation will not change already used TPPs

Dynamic interpolation (table look up)

- Grid and interpolation should take into account
  - Thermodynamic relations between TPPs (for derivatives for example) and their typical (monotonic) behavior vs parameters change (**thermodynamic consistency**)
  - Type of fluid (one-component, multicomponent, pseudo-components – petroleum fractions)
  - Parameter region vs Phase diagram of fluid (critical point and gas-liquid envelope)
    - Interpolate inside region with curved boundaries (saturation line, envelop)
  - Type of fluid flow calculation in Hydrosystem (needed TPPs)
  - Features of specific Thermal PMC
    - Can it do PE and TPP vs (p, h) or (p, s) or only (p, T)
    - Can it calculate derivatives?

Dynamic interpolation (table look up)

- Many CAPE software vendors probably do this internally – but keep it as Know-how
- Surprisingly limited number of scientific articles
- **We want to find, implement and publish universal approach** how to do this!
  - Optimal grids
  - Interpolation methods
  - Accuracy estimation vs # of point, type of fluid and region in Pr, Tr
- **This is the research topic of Maria Scripachenko research for her PhD in computer science and engineering**
- Initial (more simple) cases (Sat. line; gases; liquids) are already partly studied
- **Any recommendations will be highly appreciated!**

Grid and Interpolation

- Hermite-type spline interpolation
  - Piecewise Cubic Hermite splines (PCHIP)
  - Monotonic Modified Akima cubic splines (Makima)
  - Classical “not-a-knot” cubic splines (Spline) for comparison
- Bicubic cubic splines for 2 dimensional regions of similar types
- Grid in appropriate dimensionless coordinates
  - Pr, Tr (ln Pr where reasonable)
- Type of grids
  - Uniform
  - Roots of Chebyshev polynomials
- Thermo PMCs used so far
  - ProSim Simulis Thermodynamics
  - STARS (PSRE Co)
  - GERG-2008 (from Prof. Wagner)
  - WaterSteamPro (IAPWS-IF97)
  - More to be added (NIST REPPROP; Calcep PVTSim; others available)

Interpolation of TPPs

> 35 one-component substances was considered:

- inorganic and organic (including heavy hydrocarbons)
- non-polar and polar
- simple and complex
- taking into account the non-sphericity of the molecule cluster formation
- Simple / complex substances were analyzed; light / heavy HC; acids / alcohols / ketones / aldehydes, saturated hydrocarbons / with double, triple bonds, cyclic and aromatic

Interpolation of TPPs on saturation line

- Number of points for experiment: 4 and 10
- Method interpolation:
    - ✓spline
    - ✓makima
    - ✓Pchip
- Grid - uniform on Pr
- TPPs on the saturation line were interpolated

Results (Saturation line)

- Optimal number of points: 10
- The best method for the number of results is an error < 1% - Spline
- The average maximum error for pchip : spline : makima is 0.30%: 0.29%: 0.29% for the error < 1%
- For TPP with a maximum error greater than 1%, the logarithm of TPP was interpolated, which helps to significantly decrease in the error

Cubic interpolation for oil fraction

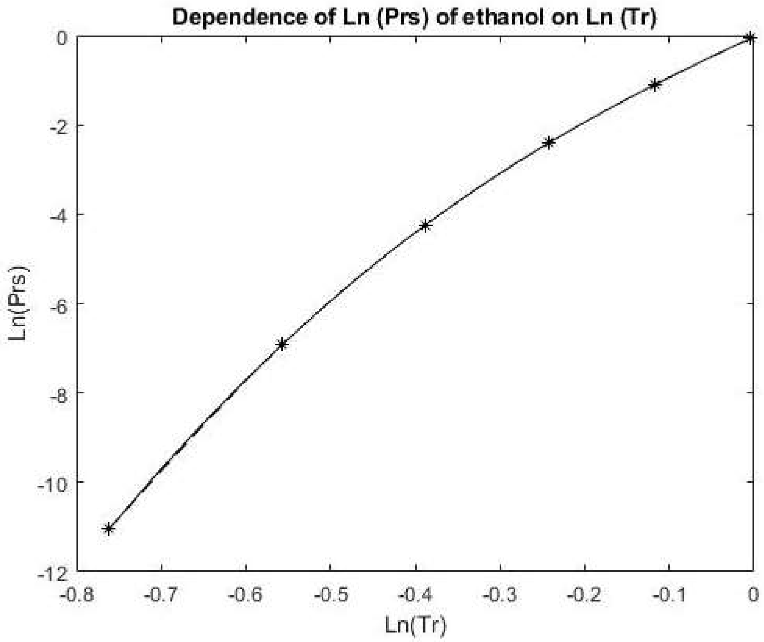


Fig. 1 The graph of the dependence of the natural logarithm of the reduced pressure of saturated vapor of the oil fraction on temperature

Derivative application. Clapeyron-Clausius equation

Accuracy without the use of a derivative = 0.21%
Accuracy with the use of a derivative = 0.011%

One phase bicubic interpolation

- Regions:
  - Subcritical Liquid: 0.41<= Pr <= 0.8; 0.6<= Tr <= 0.75
  - Gas: 0.01<= Pr <= 0.3; 0.7<= Tr <= 0.9
  - Supercritical: 1.03<= Pr <=1.80; 1.2<= Tr <=1.8
- Interpolation in MATLAB.
- Bicubic splines:
  - Modified Akima (makima)
  - not-a-knot spline
- Grid: Uniform via Pr, Tr
- Mesh size: 4x4 and 10x10

Results (one phase fluid)

Optimal mesh size: 10 x 10

- For liquids: Makima
- For the subcritical gas: Makima
- For the supercritical fluid: Spline
- The average maximum error is 0.4% for results less than 1%
- For TPPs with a maximum error greater than 1%, the logarithm of TPP was used for interpolation, and this helps to a decrease the error

Conclusion

- **Application of bicubic splines allows to interpolate TPP of real gases and liquids with high accuracy in wide ranges of pressure and temperature changes.**
- **In most cases, natural splines give slightly better accuracy than modified Akima splines, however, when approaching the critical point, when the change in the interpolated value is very uneven, the use of the latter, as well as the interpolation of the logarithm of the property value, can significantly increase the interpolation accuracy.**
- **Numerical analysis of the required number of calls in comparison with the cost of building splines indicates the advisability of using the spline interpolation method, since the results of such calculations are in good agreement with the data of thermodynamic libraries and can be used in engineering practice.**

Next steps

- Complex multicomponent fluids TPPs interpolation
- 2D Interpolation inside gas-liquid envelop
- Interpolated representation of phase diagram boundaries
- Interpolation in the regions with curved boundaries
- Special interpolation near fluid critical point

- Any other proposals?

- **Great thanks to our VP on IT Alexey Timoshkin for his very useful assistance and recommendations!**

Thank you!

Any questions?

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