




# Přehled SW pro výpočty fázových rovnováh



# SW pro metodu CALPHAD

	Thermo- Calc	MTDATA	Chem- Sage	Lucas program package	PD-pp program package
Trade mark					PD-pp
required USER education	M.S. engineer, * advanced thermody- misticist	M.S. engineer	M.S. engineer	very advanced thermodynamicist and good programer	M.S. engineer or thermo- dynamicist
U T I L I T Y	calculation of equilibria	Yes	Y	Y	Y
	Data bank	Y	Y	Y	N
	Graphical output	Y	Y	Y	N
	extracting of TD-parameters from exp. results	* Y	N	N	Y
hardware & software requirement	UNIX (VAX)	VAX (UNIX) 386/486 MSDOS PCs	PC ≥ 386	PC ≥ 486 (DOS)	PC ≥ 286 (+MS) WIN.
Origin	Sweden	UK	AACHEN	STUTGARD	CZECH R.
price [DM]	10000-15000 (annual)	9000-13000 (annual)	9400-8000,- 2000-1000,- (multi lic.)	-publication -reference [Lucas]	TD-parameters (* .pat file)

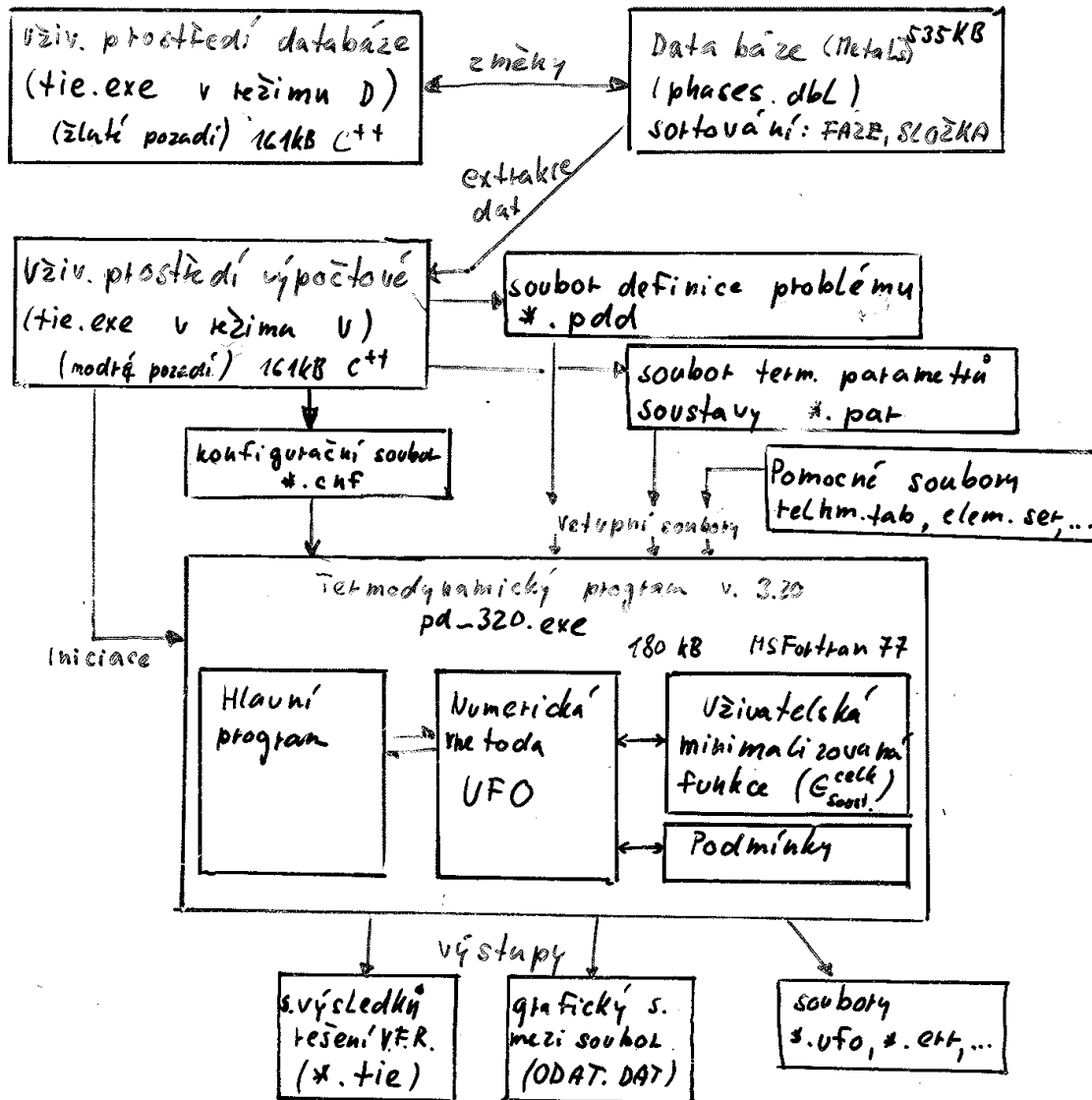


<http://www.computerherm.com/>



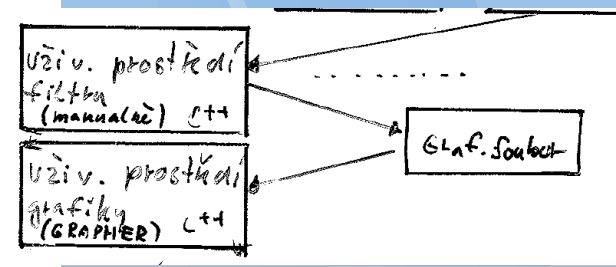
<http://gtt.mch.rwth-aachen.de/gtt-web/factsage>

# PD-PP (Phase diagram programme package)



PD-pp:  
 - 4 phases, 8 comp.  
 - activities, chem. pot., phase ratio, ...)

- sublattice model (4. subl.)  
 - integral. cond.  
 - Linear constraints



# ThermoCalc

Databáze: KP, Geo, SALT, SLAG, ION, Fe-data

DATA  
(databáze  
a tvorba TPS)

POLY-3  
(výpočet FD)

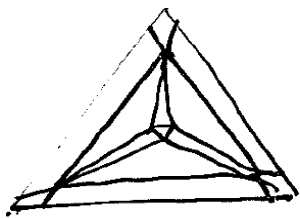
Num. metoda pro řešení integrační podm FR  
(není prezentováno)

POST (Grafika)

GES, TABULATE,  
ata.

Parrot  
(assessment FD)

Uset modals



Pozn.: "DIKTRA" - modul pro výpočty difúzních koeficientů z TP.

# Výpočtové SW a DATABASES pro chemickou termodynamiku

Name	Host	Content	Access Mode
FACT	École Polytechnique de Montréal	Integrated thermochemical database which couples software with thermodynamic data.	online, PC and web
THERDAS	Lehrstuhl für Theoretische Hüttenkunde	Databank system for thermochemical data	PC-disks, non-commercial
Thermoalloy	THERMODATA <a href="http://thermodata.online.fr/anglais.html">http://thermodata.online.fr/anglais.html</a>	Properties of multicomponent systems, and phase diagrams	Transpac, Internet
Thermo-Calc	Royal Institute of Technology	Software for thermodynamic and phase diagram calculations, specially designed for systems with strongly non-ideal phases.	PC and workstation

## DATABASES pro chemickou termodynamiku

Name	Host	Content	Access Mode
Thermophysical and Thermochemical Property Database	JICST. factual databases (JOIS-F)	thermophysical and related data for inorganic and low molecular weight compounds and up to 3-component systems.	planned for WWW, subscript. Note: this service is temporary down
<u>KINDAS</u>	Lehrstuhl für Theoretische Hüttenkunde	Database of kinetic properties and with calculation programs	PC-disks, commercial
<u>THERDAS</u>	Lehrstuhl für Theoretische Hüttenkunde	Databank system for thermochemical data	PC-disks, non-commercial
Thermocomp	<u>THERMODATA</u>	Thermodynamic properties of elements and substances in inorganic chemistry, and their reactions.	Transpac, Internet

# Další užitečné linky

**ThermoCalc (Švédsko):**

<http://www.thermocalc.com/>

**MTData (Velká Británie):** <http://www.npl.co.uk/advanced-materials/measurement-techniques/modelling/mtdata>

**FactSage (Canada+SRN)** <http://www.factsage.com/> (i příklady diagramů), Downloady:  
<http://www.crct.polymtl.ca/fact/download.php#>

**Pandat (USA, Japan, Corea):** <http://www.computherm.com/home.html>

**THERMODATA (Francie)** <http://thermodata.online.fr>

**VLXE (polymery) free:** <http://www.vlxe.com>

**Diagramy:**

**ASM :** <http://www.asminternational.org/asmenterprise/apd/default.aspx> , MSI (Ize koupit si diagram)

**Databaze**

**STGE** <http://www.crct.polymtl.ca/sgte/index.php>

**Assessment**

**Kniha:** <http://www.springerlink.com/content/100270622k03vo66/>

# Diskuse

<http://thermodata.online.fr/nuclea.html>