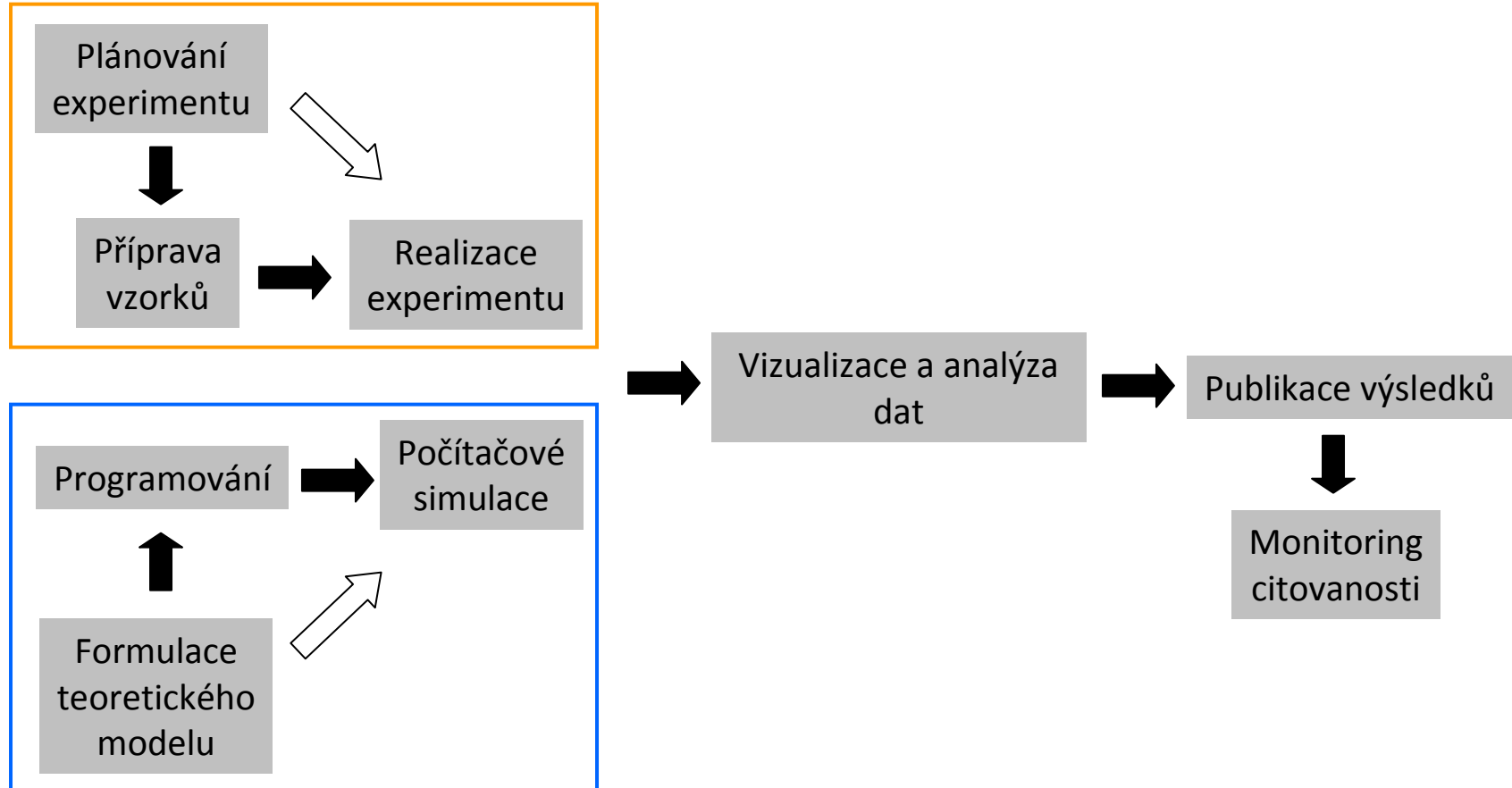




Základní nástroje vědecké práce aneb *Nechte počítače počítat*

Roman Gröger

Typický postup vědecké práce



Nástroje pro publikační činnost (cca 45 min)

Jak být informován o nových publikacích v mé vědní oblasti?

Jak získávat upozornění na citace mých článků?

Jak si vytvořit databázi článků s linky k jednotlivým PDF souborům?

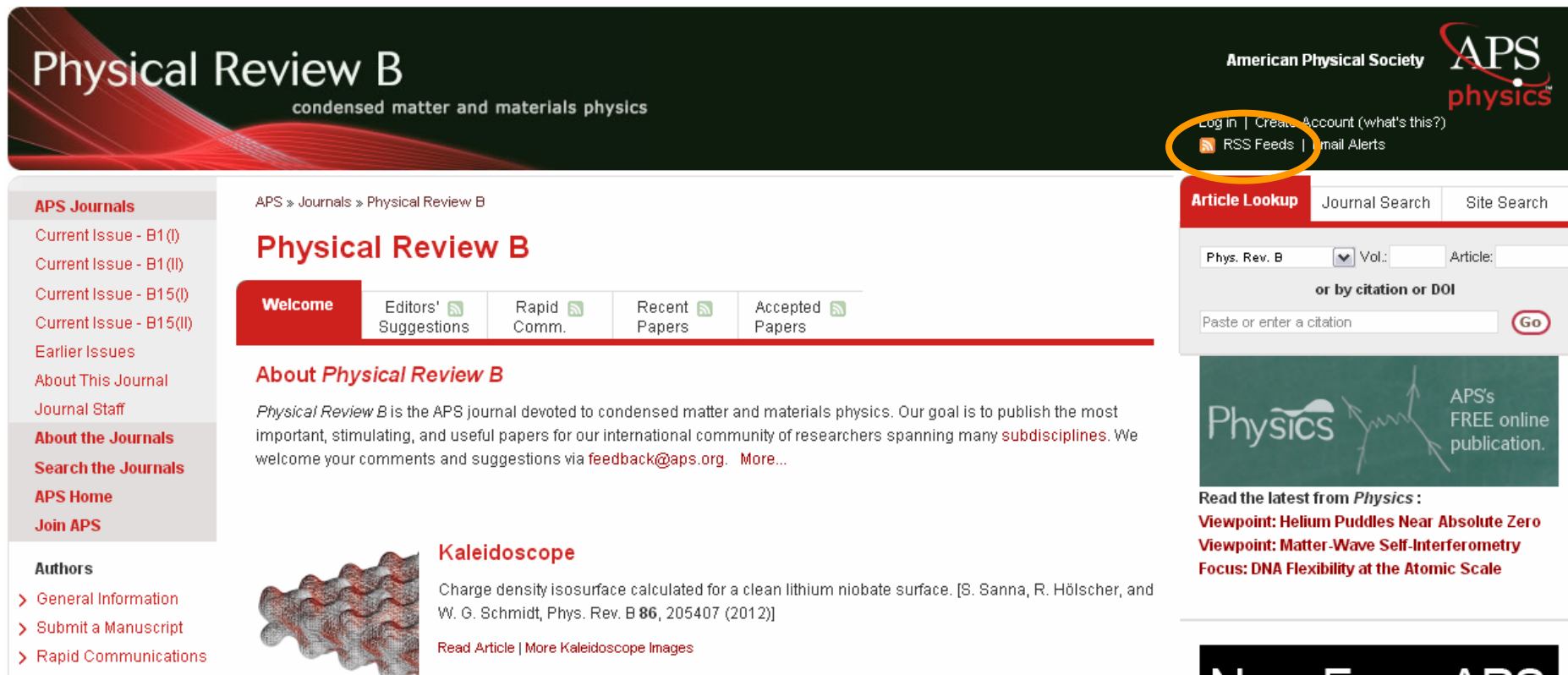
Jak používat tuto databázi při psaní článků (ve Wordu i v LaTeXu)?

Co je to vůbec LaTeX a v čem je lepší než Word?

RSS kanály

Wikipedia:

“Technologie RSS umožňuje uživatelům Internetu přihlásit se k odběru novinek z webu, který nabízí RSS zdroj (*RSS feed*, též RSS kanál, *RSS channel*). Tento zdroj se většinou vyskytuje na stránkách, kde se obsah mění a přidává velmi často (například zpravodajské servery).”

A screenshot of the Physical Review B website. The header features the journal title "Physical Review B" and the subtitle "condensed matter and materials physics" on the left, and the American Physical Society (APS) logo on the right. In the top right corner, a navigation bar includes links for "Log in", "Create Account (what's this?)", "RSS Feeds" (which is circled in orange), and "Email Alerts". Below the header, the left sidebar contains a list of links under "APS Journals" and "About the Journals". The main content area has a "Welcome" section with links to "Editors' Suggestions", "Rapid Comm.", "Recent Papers", and "Accepted Papers". Below this is a section titled "About Physical Review B" with a paragraph about the journal's focus and a link to "feedback@aps.org". Further down, there is a "Kaleidoscope" section featuring a 3D visualization of a charge density isosurface and a link to "Read Article | More Kaleidoscope Images". On the right side, there is an "Article Lookup" section with search fields for "Phys. Rev. B", "Vol.", and "Article", and a "Go" button. Below the search section is a banner for "Physics" with the text "APS's FREE online publication." and a list of recent articles under the heading "Read the latest from Physics".

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- doporučení článků od ostatních čtenářů
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Analyzing threshold pressure limitations in microfluidic transistors for self-regulated microfluidic circuits

Sung-Jin Kim, Ryuji Yokokawa, and Shuichi Takayama This paper reveals a critical limitation in the electro-hydraulic analogy between a microfluidic membrane-valve (μ MV) and an electronic transistor. Unlike typical transistors that have similar on and ...

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cond-mat.mtrl-sci (279)

Channeling of a sub-angstrom electron beam in a crystal mapped to two-dimensional molecular orbitals. (arXiv:1212.1154v1 [cond-mat.mtrl-sci])

The propagation of high-energy electrons in crystals is in general a complicated multiple scattering problem. However, along high-symmetry zone axes the problem can be mapped to the time evolution of a two-dimensional (2D) molecular system. Each ...

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Thermodynamical Property of Entanglement Entropy for Excited States. (arXiv:1212.1164v1 [hep-th])

We argue that the entanglement entropy for a very small subsystem obeys a property which is analogous to the first law of thermodynamics when we excite the system. In relativistic setups, its effective temperature is proportional to the inverse of ...

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High Energy Physics - Experiment

Measurement of the neutrino velocity with the OPERA detector in the CNGS beam

The OPERA Collaboration: T. Adam, N. Agafonova, A. Aleksandrov, O. Altinok, P. Alvarez Sanchez, A. Anokhina, S. Aoki, A. Ariga, T. Ariga, D. Autiero, A. Badertscher, A. Ben Dhabbi, A. Bertolin, C. Bozza, T. Brugiere, R. Brugnera, F. Brunet, G. Brunetti, S. Buontempo, B. Carlus, F. Cavanna, A. Cazes, L. Chaussard, M. Chernyavsky, V. Chiarella, A. Chukanov, G. Colosimo, M. Crespi, N. D'Ambrosio, G. De Lellis, M. De Serio, Y. Declais, P. del Amo Sanchez, F. Di Capua, A. Di Crescenzo, D. Di Ferdinando, N. Di Marco, S. Dmitrievsky, M. Dracos, D. Duchesneau, S. Dusini, T. Dzhaldoev, J. Ebert, I. Efthymiopoulos, O. Egorov, A. Ereditato, L. S. Esposito, J. Favier, T. Ferber, R. A. Fini, T. Fukuda, A. Garfagnini, G. Giacomelli, M. Giorgini, M. Giovannozzi, C. Girerd, J. Goldberg, C. Gollnitz, et al. (132 additional authors not shown)

(Submitted on 22 Sep 2011 (v1), last revised 12 Jul 2012 (this version, v4))

The OPERA neutrino experiment at the underground Gran Sasso Laboratory has measured the velocity of neutrinos from the CERN CNGS beam over a baseline of about 730 km. The measurement is based on data taken by OPERA in the years 2009, 2010 and 2011. Dedicated upgrades of the CNGS timing system and of the OPERA detector, as well as a high precision geodesy campaign for the measurement of the neutrino baseline, allowed reaching comparable systematic and statistical accuracies. An arrival time of CNGS muon neutrinos with respect to the one computed assuming the speed of light in vacuum of $(6.5 \pm 7.4(\text{stat.}) (+8.3(-8.0)\text{sys.}))\text{ns}$ was measured corresponding to a relative difference of the muon neutrino velocity with respect to the speed of light $(v-c)/c = (2.7 \pm 3.1(\text{stat.}) (+3.4(-3.3)\text{sys.})) \times 10^{-6}$. The above result, obtained by comparing the time distributions of neutrino interactions and of protons hitting the CNGS target in 10.5 microseconds long extractions, was confirmed by a test performed at the end of 2011 using a short bunch beam allowing to measure the neutrino time of flight at the single interaction level.

Comments: 34 pages, 22 figures This version replaces all previous ones

Subjects: **High Energy Physics - Experiment (hep-ex)**; High Energy Physics - Phenomenology (hep-ph)

Cite as: arXiv:1109.4897 [hep-ex]
(or arXiv:1109.4897v4 [hep-ex] for this version)

Submission history

From: Laura Patrizi [[view email](#)]

[v1] Thu, 22 Sep 2011 17:59:33 GMT (4763kb)
[v2] Thu, 17 Nov 2011 11:17:26 GMT (6498kb)
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Organizace článků

www.endnote.com



EndNote (komerční, Windows)

- v současnosti nejpopulárnější reference manager pro Word

The screenshot shows the EndNote 6 interface. The main window displays a list of references with columns for Author, Year, and Title. The list includes references by Groma (1997, 1999, 2003, 2006, 2007), Grujicic (1997), Gschneidner Jr. (1963), Guiton (2007), Guiu (1966, 1967, 1968, 1969), Gulluoglu (1989), Gumbsch (1999, 2001), Gunton (1974), Guo (2003), Gupta (1997, 1999, 2007), Gurtin (1966), Gushchin (1984), Haataja (2004, 2005, 2005), Hachiya (1999), Hackenberger (2001), Haeni (2004), Hale (1991), Hall (1967), Halley (2002), and Hamermesh (1989).

A detailed view of a reference is shown in the foreground window, titled "Riemann, 1859 #1556". The reference type is "Journal Article". The fields are filled with the following information:

- Author:** Riemann, B.
- Year:** 1859
- Title:** On the number of prime numbers less than a given quantity
- Journal:** Monatsberichte der Berliner Akademie
- Volume:**
- Issue:**
- Pages:**
- Date:** 1859
- Short Title:**
- Alternate Journal:**

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#	Entrytype	Author	Title	Year	Journal	Bibtexkey
1	Book	{von Neumann}	Vorlesungen \u00fcber die Theorie der Elastizit\u00e4t	1885		neumann:18...
2	Article	d'Almeida and Gupta	Real-time X-ray diffraction measurements of the phase t...	2000	Phys. Rev. Le...	dalmeida:00
3	Article	\Osterle et al.	Modelling the orientation and direction dependence of th...	2000	Acta Mater.	osterle:00
4	Article	\Ottinger	Lie groups in nonequilibrium thermodynamics: {G}eometri...	2010	J. Non-Newto...	ottiger:10
5	Electronic	{\it efunda.com}	Thermal conductivity of copper. {\tt http://www.efunda.co...	2011		efunda-kapp...
6	Article	\v{S}est\u00e1k	Modern aspects of plastic deformation in metals	1972	Czech. J. Phy...	sestak:72
7	Inbook	\v{S}ob	Multiscale materials modelling: {F}undamentals and appli...	2007		sob:07
8	Article	Abers and Lee	Gauge theories	1973	Phys. Rep.	abers:73
9	Article	Acebr\u00f3n et al.	The {K}uramoto model: {A} simple paradigm for synchron...	2005	Rev. Mod. Ph...	acebron:05
10	Article	Achar and Barsch	Anharmonicity and mode softening in {Nb}_{3}Sn	1981	Phys. Rev. B	achar:81
11	Article	Achar and Barsch	Anharmonic contribution to mode softening in {V}_{3}Si	1979	Phys. Rev. B	achar:79
12	Article	Acharya	Constitutive analysis of finite deformation field dislocatio...	2004	J. Mech. Phys...	acharya:04
13	Article	Acharya	A model of crystal plasticity based on the theory of contin...	2001	J. Mech. Phys...	acharya:01
14	Article	Acharya et al.	New perspectives in plasticity theory: dislocation nucleatio...	2008	Math. Mech. ...	acharya:08
15	Article	Acharya and Roy	Size effects and idealized dislocation microstructure at sm...	2006	J. Mech. Phys...	acharya:06
16	Article	Acharya and Shawki	Clausius-{D}uhem inequality and the structure of rate-ind...	1996	Int. J. Plast.	acharya:96
17	Article	Ackermann et al.	Temperature and strain-rate dependence of the flow stre...	1983	Acta Metall.	ackermann:83
18	Article	Ackland	Simulation of martensitic microstructure	2005	J. Mater. Sci.	ackland:05
19	Article	Ackland	Theoretical study of the effect of point defects on the ela...	1988	J. Nucl. Mater.	ackland:88
20	Article	Ackland and Pinsook	How do martensitic twin boundaries move?	2002	Mat. Res. So...	ackland:02
21	Article	Ackland and Reed	Two-band second moment model and an interatomic pote...	2003	Phys. Rev. B	ackland:03
22	Article	Ackland and Thetford	An improved N-body semi-empirical model for body-centre...	1987	Philos. Mag. A	ackland:87
23	Techreport	Adams and Oetting	The chemical thermodynamics of nuclear materials	1982		adams:82
24	Article	Addessio et al.	Model for high-strain-rate deformation of uranium-niobium...	2003	J. Appl. Phys.	addessio:03
25	Article	Adler and Olson	Thermodynamics and kinetics of $\delta \rightarrow \gamma$	1988	Metall. Trans...	adler:88
26	Article	Aguirre et al.	Fractal structures in nonlinear dynamics	2009	Rev. Mod. Ph...	aguirre:09
27	Article	Ahart et al.	Origin of morphotropic phase boundaries in ferroelectrics	2008	Nature	ahart:08
28	Article	Ahlgren et al.	Bond-order potential for point and extended defect simula...	2010	J. Appl. Mech.	ahlgren:10
29	Article	Ahluwalia and Cao	Influence of dipolar defects on switching behavior in ferro...	2001	Phys. Rev. B	ahluwalia:01
30	Article	Ahluwalia et al.	Dynamic strain loading of cubic to tetragonal martensites	2006	Acta Mater.	ahluwalia:06
31	Article	Ahluwalia et al.	Landau theory for shape memory polycrystals	2004	Acta Mater.	ahluwalia:04
32	Article	Ahluwalia et al.	Domain-size dependence of piezoelectric properties of ferr...	2005	Phys. Rev. B	ahluwalia:05
33	Article	Ahluwalia et al.	Piezoelectric response of engineered domains in ferroelec...	2004	Appl. Phys. L...	ahluwalia:04a
34	Article	Ahn et al.	Ferroelectricity at the nanoscale: {L}ocal polarization in o...	2004	Science	ahn:04
35	Article	Ahn et al.	Local, nonvolatile electronic writing of epitaxial {Pb}(Zr_{x}...	1997	Science	ahn:97
36	Article	Ahn et al.	Atomic scale lattice distortions and domain wall profiles	2002	Phys. Rev. B	ahn:02

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- unikátní označení vědce, např. G-3608-2010 (já)

The screenshot shows a web browser window with the ResearcherID profile of Roman Gröger. The browser tabs include 'Condensed matter theory ar', 'Roman Gröger G-3608-2010', and 'ResearcherID Labs'. The address bar shows 'www.researcherid.com/rid/G-3608-2010'. The page header features the ResearcherID logo and Thomson Reuters branding. Navigation links include Home, Login, Search, Interactive Map, and EndNote Web. The profile section for Roman Gröger (G-3608-2010) includes a URL, subject (Materials Science, Mathematics, Mechanics, Physics), and keywords (dislocations, atomistic modeling, phase field, point defects, eshelby twist, peierls barrier, thermodynamics, statistical mechanics, monte carlo method, entropy, activation energy, rare events, bond order potential, differential displacements, extended defects). It also lists his primary institution (Academy of Sciences of the Czech Republic), joint affiliation (Brno University of Technology), and past institutions (University of California, Los Angeles). A description of his research is provided, along with his website URL. On the left, a 'My Publications' sidebar shows 16 publications, with links to view them and citation metrics. The main 'My Publications: View' section shows a list of publications, with the first one being 'Bond-order potential for simulations of extended defects in tungsten' by Mrovec, M.; Gröger, R.; Bailey, A.G.; et al., published in Physical Review B in March 2007, cited 40 times. A callout box on the right highlights the top three most cited publications.

Gröger, Roman [Get A Badge](#) [ResearcherID](#) [Labs](#)

ResearcherID: G-3608-2010
URL: <http://www.researcherid.com/rid/G-3608-2010>
Subject: Materials Science; Mathematics; Mechanics; Physics
Keywords: dislocations; atomistic modeling; phase field; point defects; eshelby twist; peierls barrier; thermodynamics; statistical mechanics; monte carlo method; entropy; activation energy; rare events; bond order potential; differential displacements; extended defects

Description: Theoretical and computational studies of physical properties of materials with defects. Mesoscopic studies of radiation damage. Evolution of transitions and nonequilibrium thermodynamics in martensites and nuclear materials. Atomistic studies of extended defects in bcc metals. Synthesis of new materials.

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Primary Institution: Academy of Sciences of the Czech Republic
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16 publication(s) Page 1 of 2 [Go](#)

1. Title: Bond-order potential for simulations of extended defects in tungsten
Author(s): Mrovec, M.; Gröger, R.; Bailey, A.G.; et al.
Source: **Physical Review B** Volume: 75 Issue: 10 Published: MAR 2007
Times Cited: 40

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- 1. Bond-order potential for simulations of extended defects in tungsten**
Times Cited: 40 (*Web of Science®*)
- 2. Multiscale modeling of plastic deformation of molybdenum and tungsten: I. Atomistic studies of the core structure and glide of $1/2 < 111 >$ screw dislocations at 0 K**
Times Cited: 33 (*Web of Science®*)
- 3. Multiscale modeling of plastic deformation of molybdenum and tungsten. III. Effects of temperature and plastic strain rate**
Times Cited: 21 (*Web of Science®*)

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California Institute of Technology

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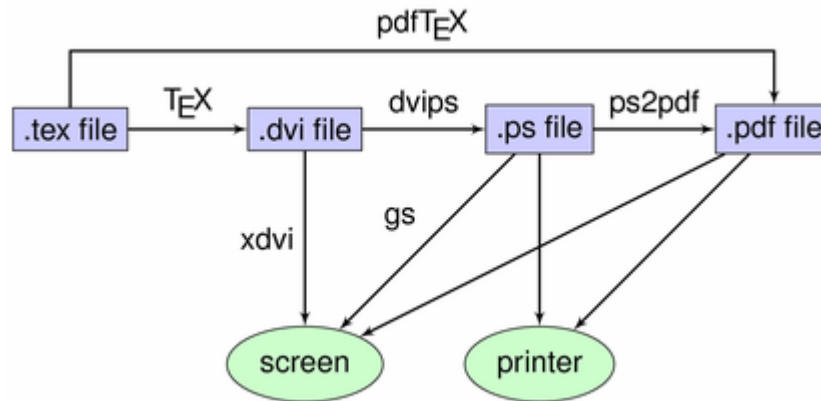
Show: 20 ▼ 1-20 Next >

Title / Author		Cited by	Year
☐ The Feynman lectures on physics	RP Feynman, RB Leighton, M Sands, SB Treiman Physics Today 17, 45	8452	1964
☐ Quantum Mechanics and Path Integrals: Emended Edition	RP Feynman, AR Hibbs, DF Styer Dover Publications	8048	2010
☐ Simulating physics with computers	RP Feynman International journal of theoretical physics 21 (6), 467-488	3175	1982
☐ Space-time approach to non-relativistic quantum mechanics	RP Feynman Reviews of Modern Physics 20 (2), 367	2861	1948
☐ There's plenty of room at the bottom	RP Feynman Engineering and Science 23 (5), 22-36	2190 *	1960
☐ Forces in molecules	RP Feynman Physical Review 56 (4), 340	2166	1939
☐ Theory of the Fermi interaction	RP Feynman, M Gell-Mann Physical Review 109 (1), 193	1855	1958
☐ Very high-energy collisions of hadrons	RP Feynman Physical Review Letters 23 (24), 1415-1417	1805	1969

LaTeX

wiki.ubuntu.cz:

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- .tex je textový formát
- velmi malý soubor (jen text + odkazy na obrázky)
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- k dispozici velké množství balíčků (packages)
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- respektuje typografická pravidla
- systém využívaný největšími nakladateli vědeckých publikací

Jednoduchý text:

```
\documentclass{article}

\begin{document}
  Hello World!
\end{document}
```

Hello World!

Vzorce:

```
\begin{equation}
  \rho \psi = \bm{\sigma}^e : \bm{\epsilon}^e + A^p \alpha^p - \rho T s
\label{eq:psi}
\end{equation}
```

$$\rho\psi = \boldsymbol{\sigma}^e : \boldsymbol{\epsilon}^e + A^p \alpha^p - \rho T s$$

Obrázky:

```
\begin{figure}
  \centering
  \includegraphics[scale=.7]{fig/barycentric}
  \caption{Barycentric coordinates on an equilateral triangle given by the three components of the vector  $\bm{\lambda}$  (black). The limiting values of the relative displacements  $u_{i,i+1}^z$  of the three atoms representing the three sides of this triangle are given in blue.}
  \label{fig:barycentric}
\end{figure}
```

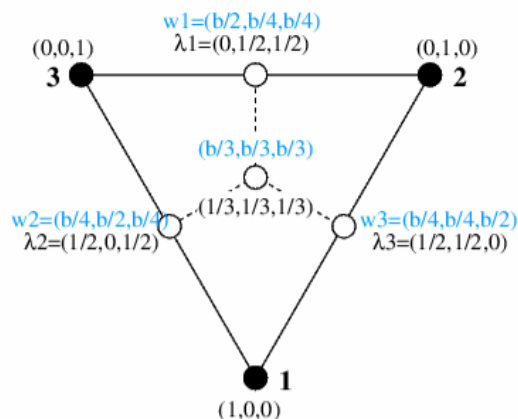


FIG. 1: Barycentric coordinates on an equilateral triangle given by the three components of the vector $\boldsymbol{\lambda}$ (black). The limiting values of the relative displacements $u_{i,i+1}^z$ of the three atoms representing the three sides of this triangle are given in blue.

Tabulky:

```
\begin{table}[!htb]
\centering
\parbox{10cm}{\caption{Coefficients of the effective yield criterion for tungsten determined by
fitting the 0~K atomistic data.}
\label{tab_tstar_params_W}}\!\!\[1em]

\begin{tabular}{cccc}
\hline
$a_1$ & $a_2$ & $a_3$ & $\tau^*_{cr}/C_{44}$ \\
\hline
0 & 0.56 & 0.75 & 0.028 \\
\hline
\end{tabular}
\end{table}
```

Table 7.1: Coefficients of the effective yield criterion for tungsten determined by fitting the 0 K atomistic data.

a_1	a_2	a_3	τ^*_{cr}/C_{44}
0	0.56	0.75	0.028

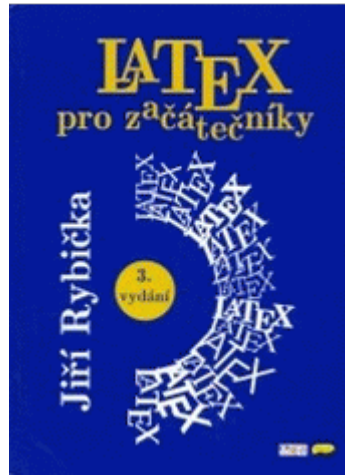
Kde ho vzít ?



<http://www.tug.org/texlive/>

Oficiální distribuce TeXu pro všechny platformy
(MacTex, teTeX, ...)

Více informací:



FI MU v Brně
Knihkupectví Mareček



Československé sdružení
uživatelů TeXu

<http://www.cstug.cz/>

“The Not So Short Introduction to LATEX 2 ϵ ”

<http://tobi.oetiker.ch/lshort/lshort.pdf>

Zpracování a vizualizace dat (cca 45 min)

Jak automatizovat rutinní operace se soubory?

Jak provádět dávkové vizualizace dat?

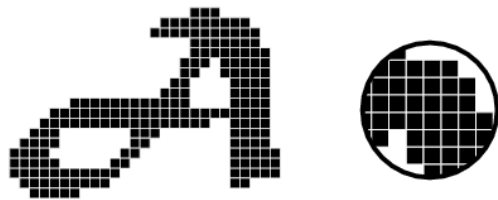
Jak zobrazit rozsáhlá 3D data a získat fotorealistický výstup?

Jak vytvářet animace a vkládat je do prezentací?

Co je to GIMP?

Bitmapová vs. vektorová grafika

vektorová grafika



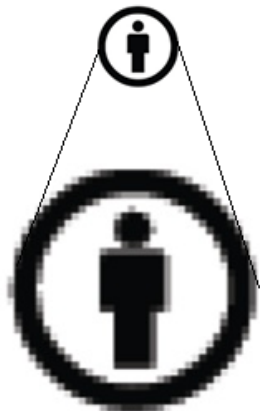
bitmapa

Vektorové formáty (výběr):

.ai	Adobe Illustrator
.cdr	Corel Draw
.emf	Enhanced Metafile
.eps	Encapsulated Postscript
.pdf	Portable Desktop Format
.pic, .pct	Macintosh PICT
.svg	Scaleable Vector Graphics
.wmf	Windows Metafiles
.ps	Postscript

Bitmapové (rastrové) formáty (výběr):

.bmp	Windows Bitmap File
.gif	CompuServe Graphics Interchange Format
.jpg	Joint Photographic Experts File
.psd	Photoshop File
.tif	Tagged-Image File Format
.xcf	eXperimental Computing Facility (GIMP)



enlarged
bitmap ("raster")



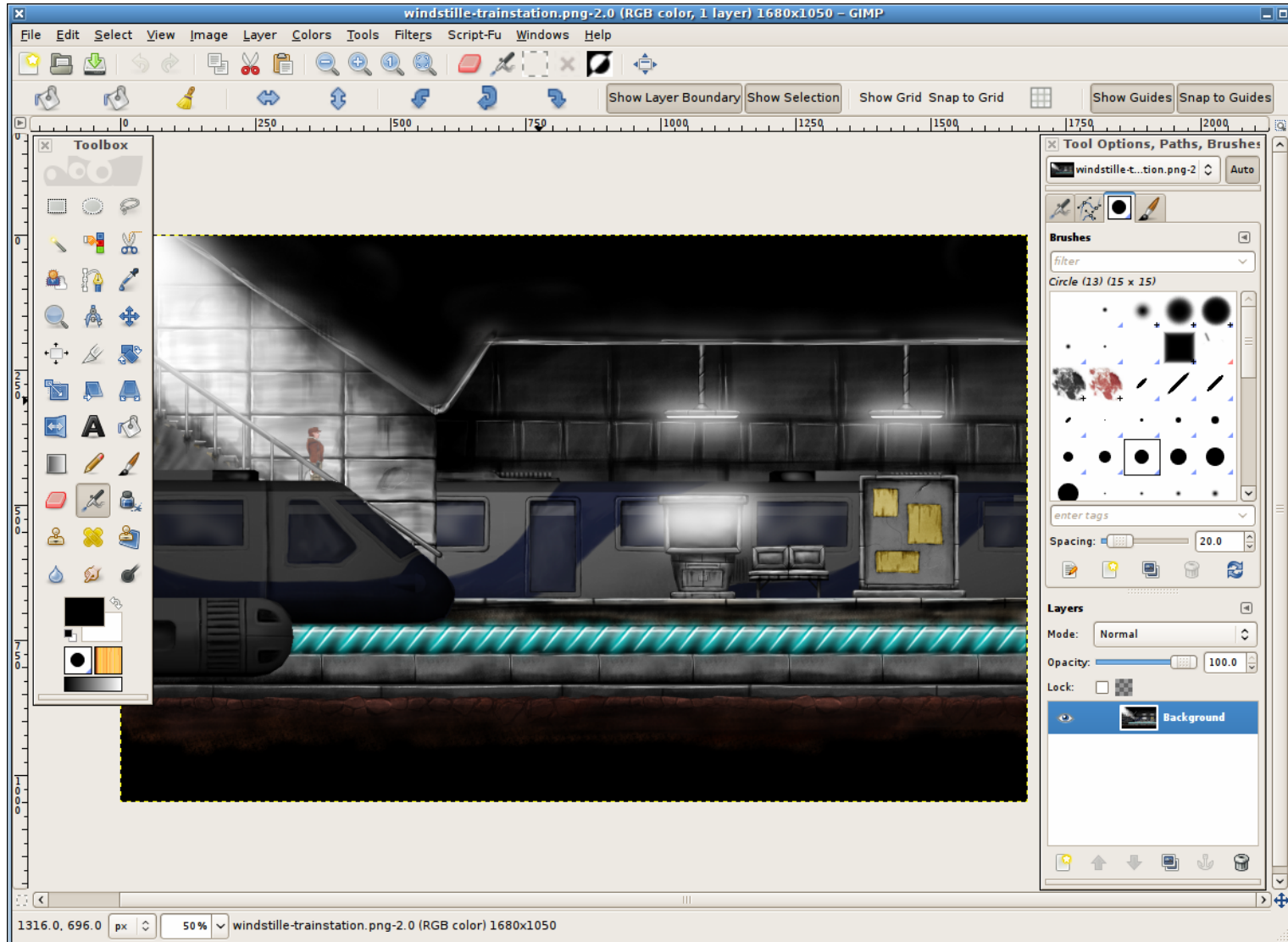
enlarged
vector

GIMP – GNU Image Manipulation Program (Windows, Mac, Linux)



www.gimp.org

Pokročilý open-source program pro vytváření, editaci a export bitmapové grafiky (s možností pozdější editace pokud je soubor uložen ve formátu .xcf)



Inkscape (Windows, Mac, Linux)

inkscape.org



Open Source editor vektorové grafiky, který má podobné funkce jako Adobe Illustrator nebo CorelDraw. Používá standardní SVG formát (Scalable Vector Graphics).

The screenshot shows the Inkscape interface with a tutorial for applying the 'Path along path' effect. The tutorial is divided into five numbered steps:

- 1 Transform shape into single path**: A fish skeleton is shown next to a plus sign and a curved line, indicating the preparation of the shape and the path.
- 2 Copy to clipboard**: A fish skeleton is shown. A note says: "(it is easiest later on to move the nose of the fish to the top-left corner of the document (0,0) before copying to the clipboard, so you don't have to manually tweak the origin parameter)".
- 3 Draw the skeleton path**: A curved line is shown, representing the path to be drawn.
- 4 Press Ctrl-Shift-7 and apply Skeletal Strokes to the skeleton path. Press the paste button next to "pattern"**: A fish skeleton is shown with a red curved line (the skeleton path) overlaid on it.
- 5 Press F2 and notice that the red skeleton path is live editable on-canvas**: A fish skeleton is shown with a red curved line (the skeleton path) overlaid on it, and a dashed box around it indicating it is live editable.

The right sidebar shows the 'Path Effects (Shift+Ctrl+7)' panel with the 'Path along path' effect selected. The 'Current effect' section shows 'Path along path' with 'Pattern copies' set to 'Single, stretched' and 'Pattern source' set to 'Clipboard'. The 'Width' is set to '1,000'. There are checkboxes for 'Width in units of length' and 'Pattern is vertical'. A 'Remove' button is at the bottom.

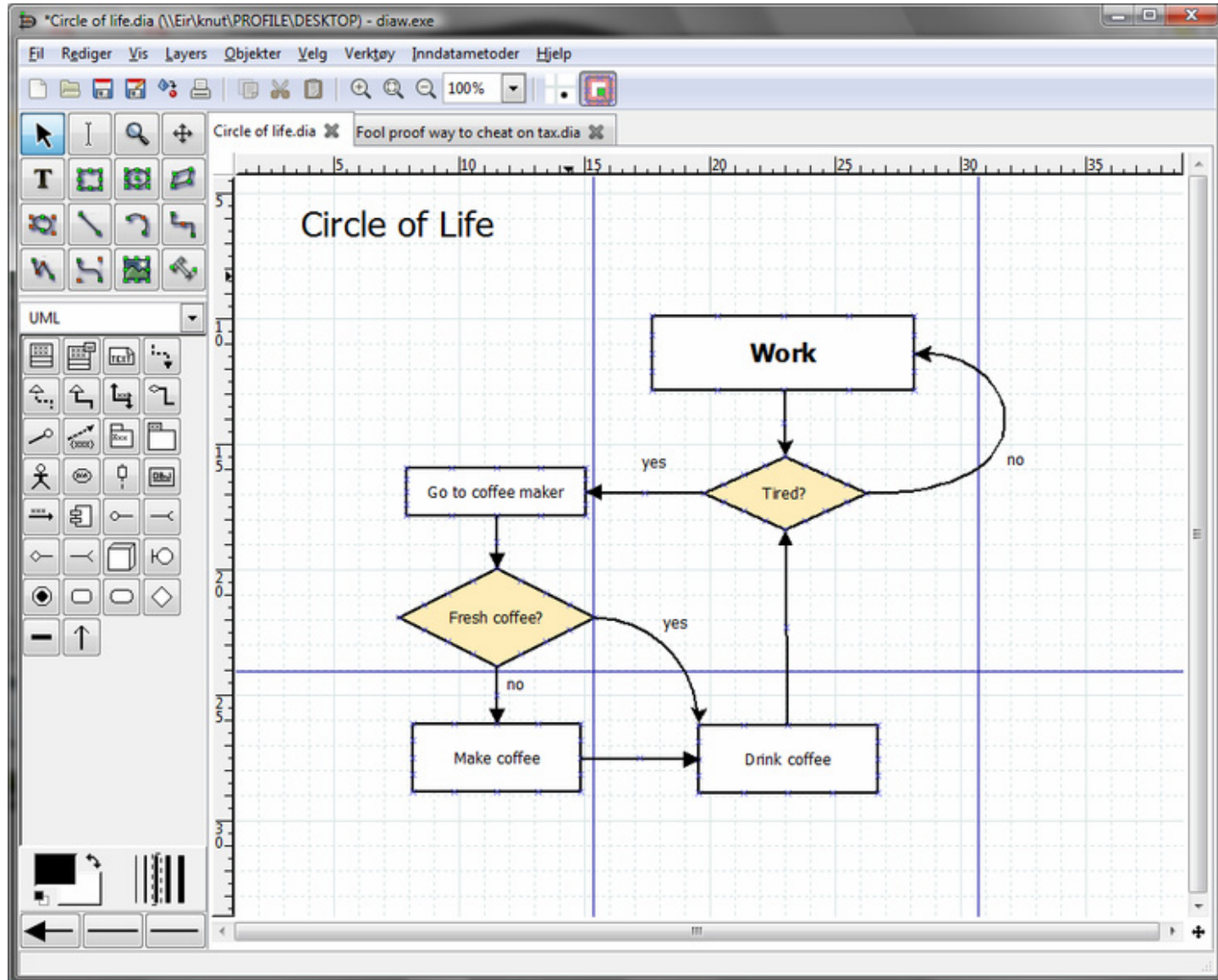
The bottom status bar shows: Fill: (empty), Stroke: 0,531, O: 100, (root), Alt: lock handle length; Ctrl+Alt: move along handles. The bottom right corner shows coordinates: X: 164,24, Y: 256,92, Z: 93%.

Dia (Windows, Mac, Linux)



Open Source vektorový grafický systém pro vytváření diagramů.

Podpora formátů XML, SVG, EPS, ...



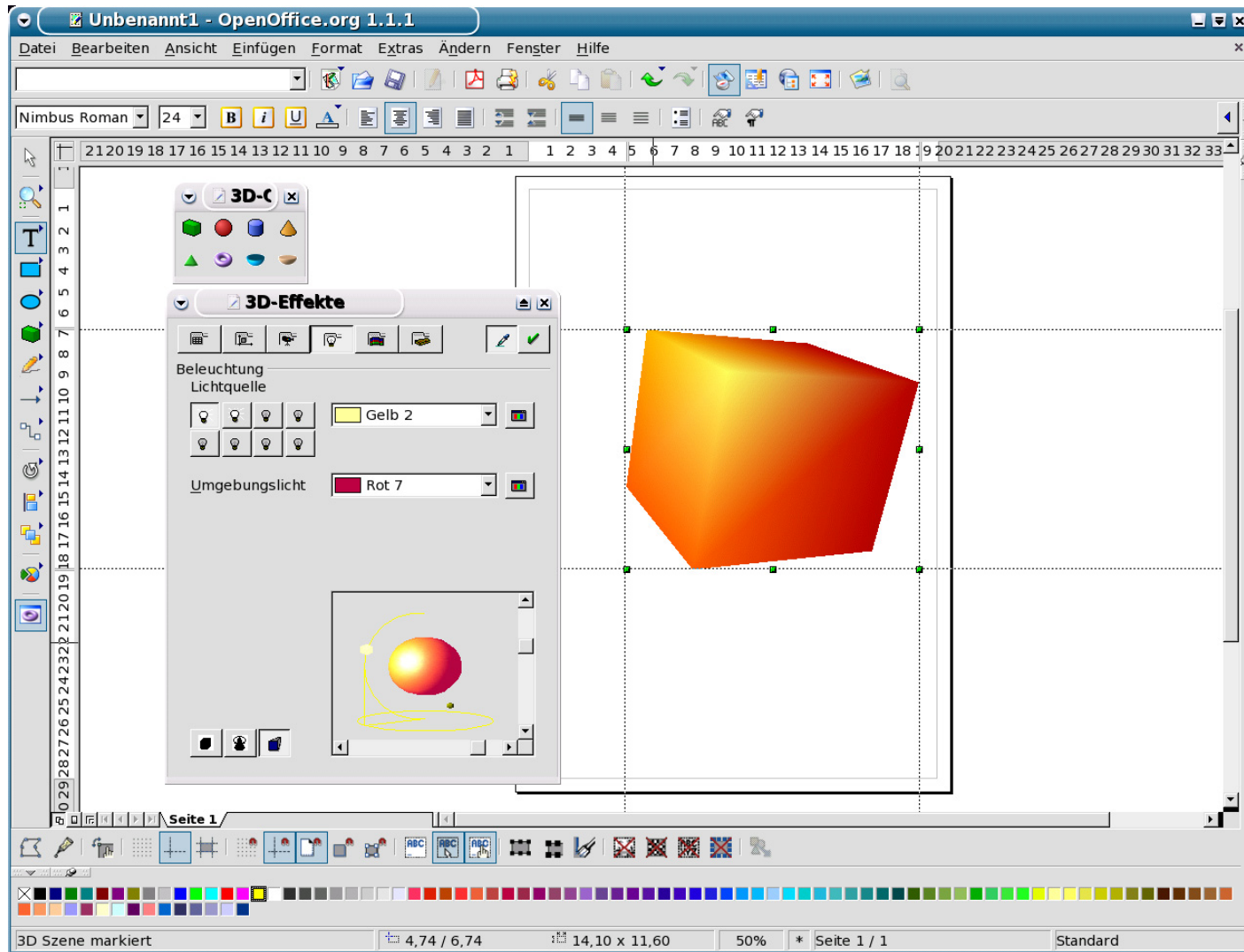
OpenOffice.org Draw (Windows, Mac, Linux)

www.openoffice.org



OpenOffice (Libre Office) je kompletní kancelářský balík.

Na rozdíl od Microsoft Office jsou oba open source a volně šiřitelné. Oba obsahují lokalizace pro drtivou většinu jazyků. OODraw je vektorový grafický editor s exportem do mnoha formátů (vč. Postscriptu).



GNU Plot (Windows, Mac, Linux)

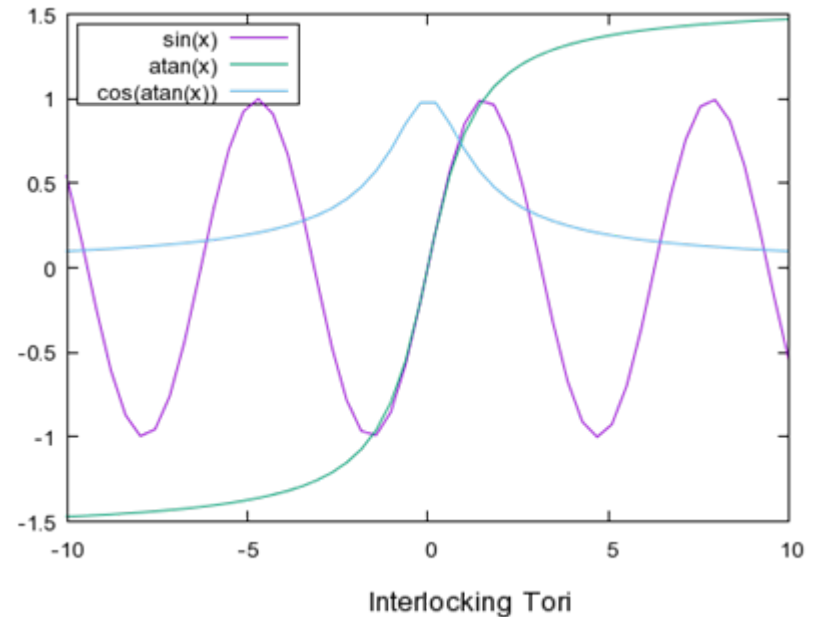
System pro dávkovou vizualizaci dat ve 2D, 3D, animace, ...

www.gnuplot.info

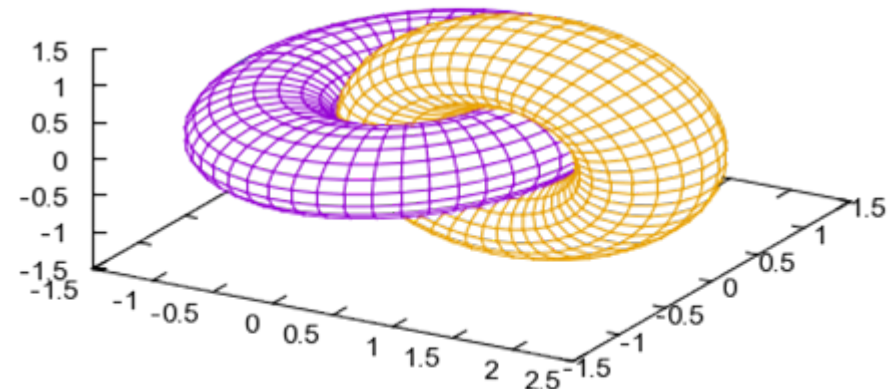


Příklady:

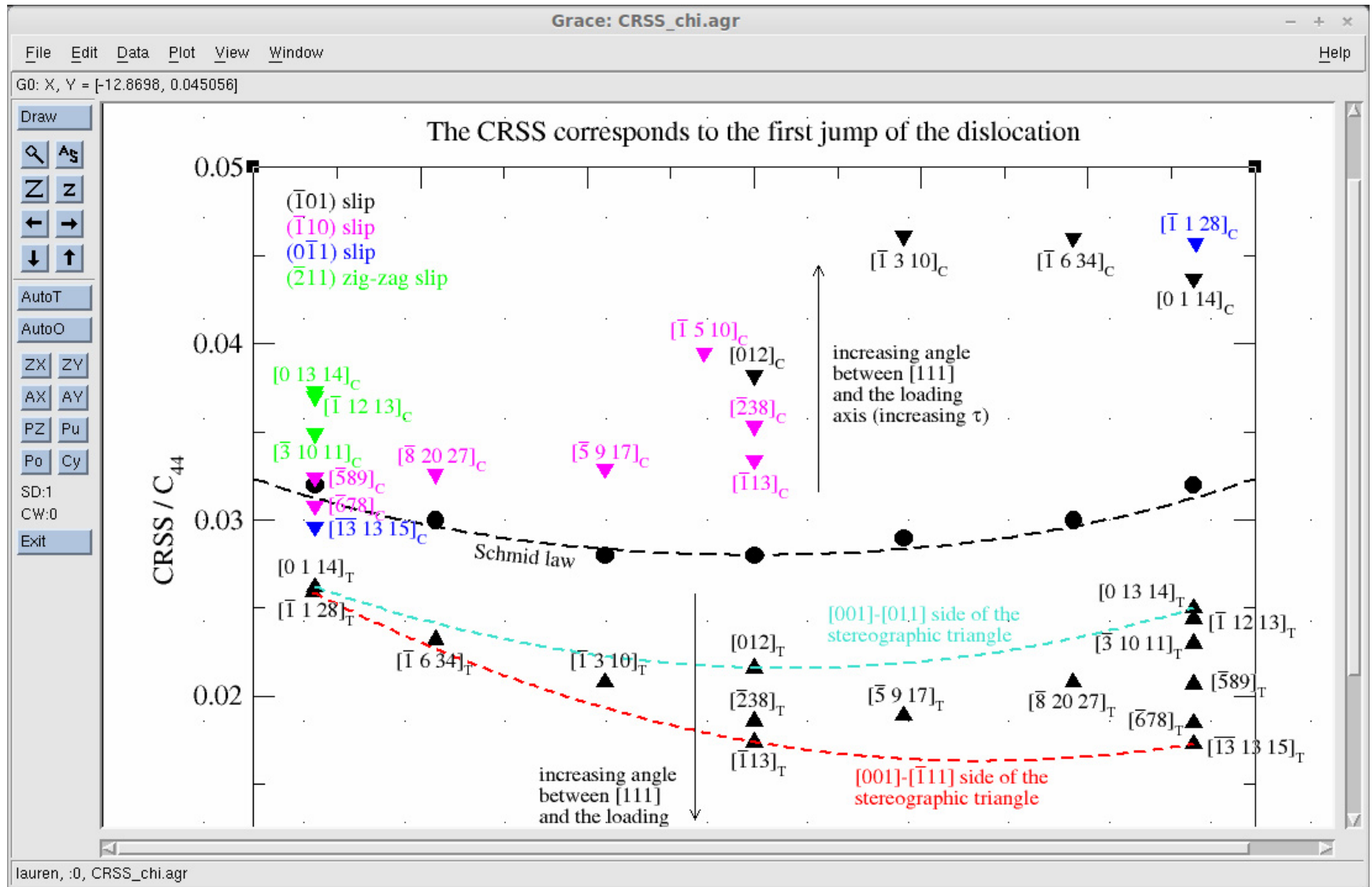
```
set key left box
set samples 50
plot [-10:10] sin(x), atan(x), cos(atan(x))
```



```
set title "Interlocking Tori"
set urange [-pi:pi]
set vrange [-pi:pi]
set isosamples 50,20
splot cos(u)+.5*cos(u)*cos(v), \
    sin(u)+.5*sin(u)*cos(v), \
    .5*sin(v) with lines, \
    1+cos(u)+.5*cos(u)*cos(v), \
    .5*sin(v), \
    sin(u)+.5*sin(u)*cos(v) with lines
```



Jednoduchý, ale hojně používaný systém pro 2D vizualizaci dat. Mimo jiné umožňuje správné psaní Millerových indexů v krystalografii !



Konverze mezi grafickými formáty



ImageMagick (Windows/Mac/Linux)

Softwarový balík (open source) k vytváření, editaci a konverzi bitmapových/vektorových souborů. Umí číst a zapisovat obrázky ve více než 100 formátech, včetně PNG, Postscript, SVG a TIFF. Jedním příkazem lze změnit velikost, zrcadlit, otáčet, deformovat, zkosit nebo transformovat, nastavit barvy, použít speciální efekty, psát text, kreslit čáry, polygony, elipsy nebo Bézierovy křivky.

Základní převod formátu:

```
convert image.gif output.png
```

Inverze obrázku:

```
convert -negate image.gif output.gif
```

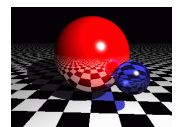
Vytvoření “halo” efektu okolo obrázku:

```
convert knight.png \( clone -channel A -blur 0x2.5 -level 0,50%  
+channel I +level-colors red  
\) -compose DstOver -composite knight_halo.png
```



Vytvoření animovaného GIFu:

```
convert -delay 20 -loop 0 sphere*.gif animatespheres.gif
```



sphere*.gif

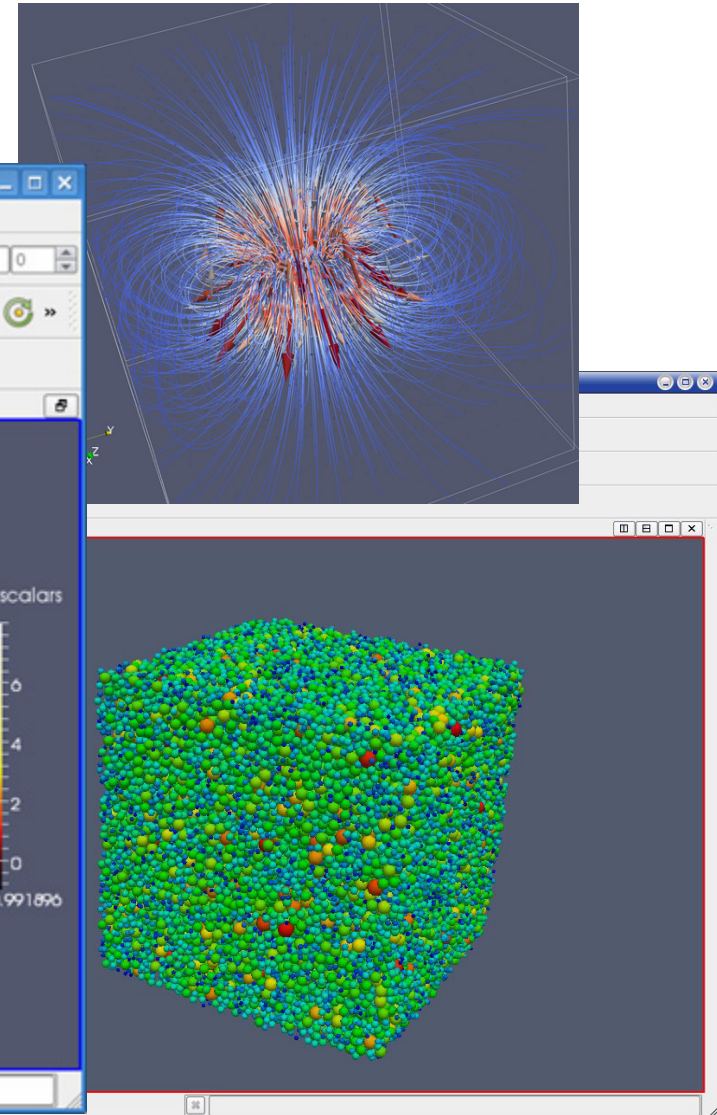
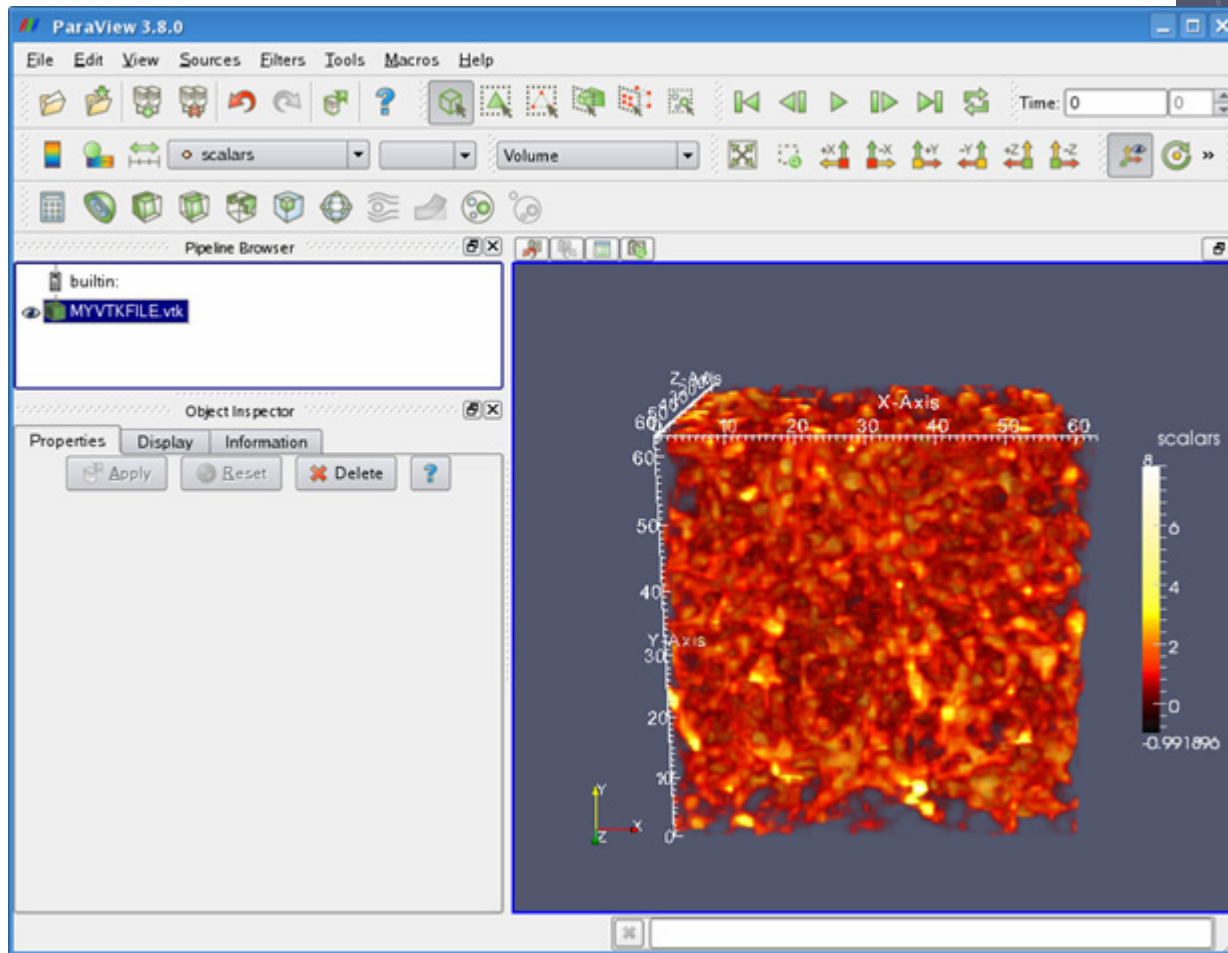
animatespheres.gif

Paraview (freeware, Windows/Mac/Linux)



Špičkový balík pro 3D vizualizaci rozsáhlých datových souborů. Fotorealistický výstup, raytracing, Postscript, animace, paralelní vizualizace, apod.

Vysoce univerzální (čte XML formát).



Open source matematický software

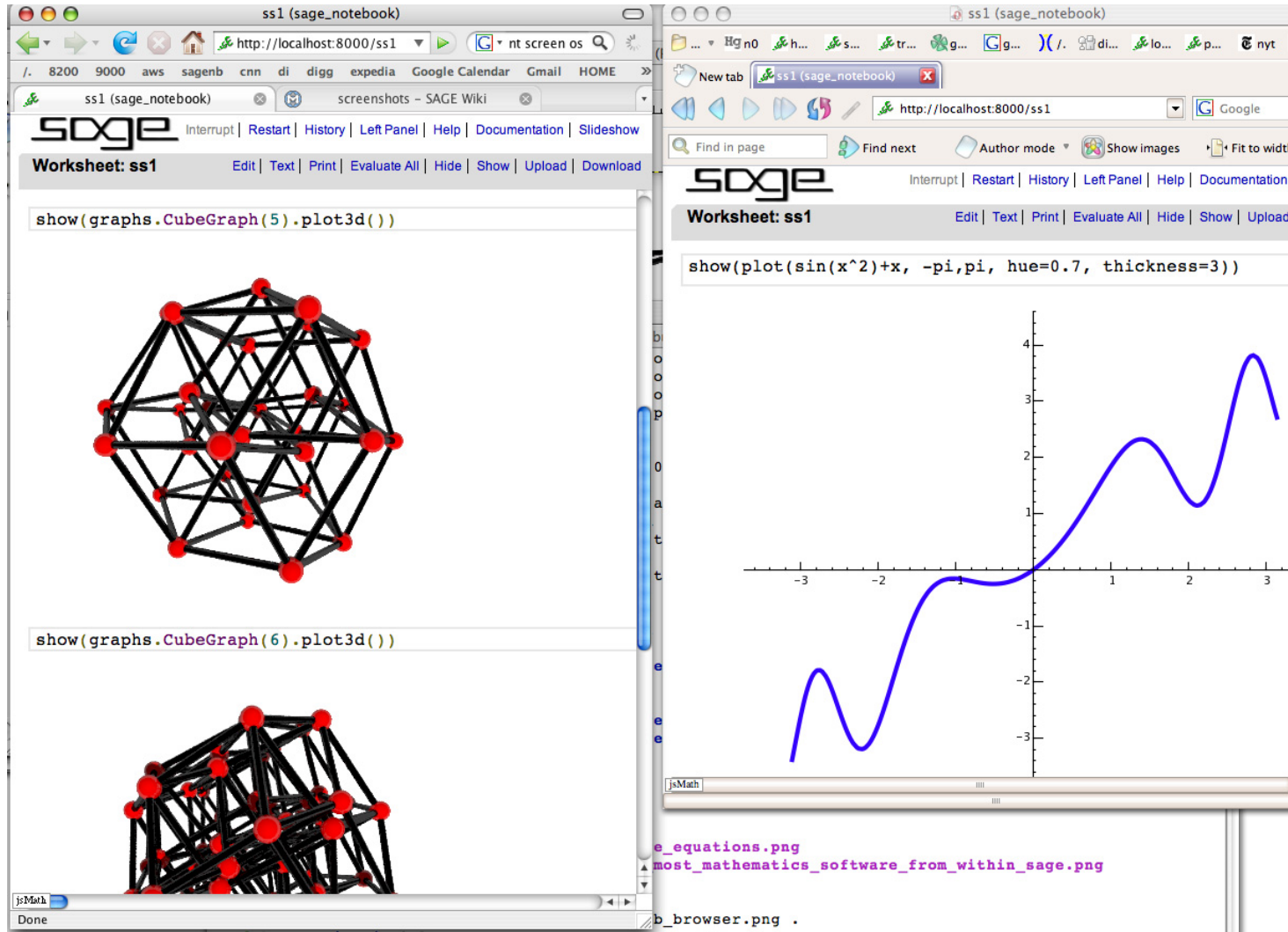


www.sagemath.org

Nejrychlejší software pro symbolickou algebru (viz. také Mathematica, Maple, Matlab)

Vysoce optimalizované algoritmy vyvíjené přímo matematiky odděleně od GUI.

Notebook běží jako webová aplikace.



Síťová komunikace a úvod do Linuxu (cca 30 min)

Základní příkazy Secure Shellu pro vzdálenou komunikaci.
Přehled skriptovacích jazyků s ukázkou použití (aneb jak jedním příkazem zpracovat celý soubor).

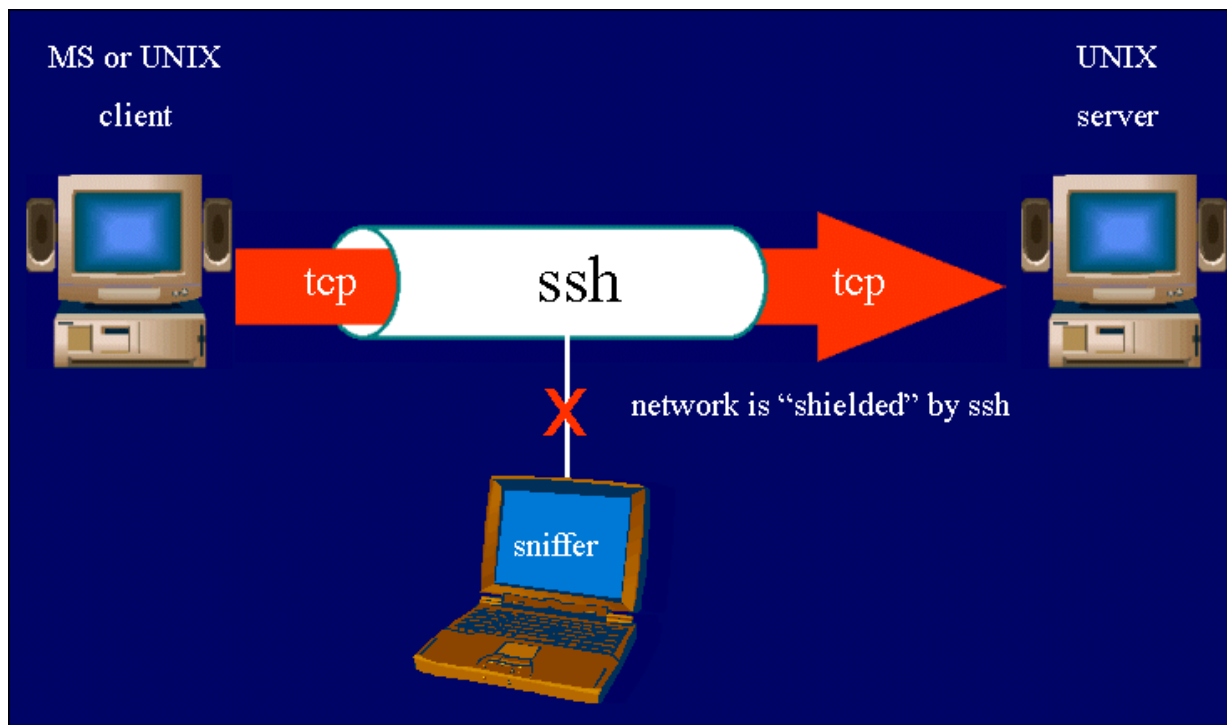
Co je to Linux a pro koho je vhodný?

K čemu jsou virtuální stroje?

Secure Shell

lokální počítač

vzdálený počítač
(např. drs.ipm.cz)



ssh protokol znemožňuje
odposlouchávání komunikace

Terminál:

PuTTY (Windows)

Terminal (Mac OS)

xterm, gnome-terminal, ... (Linux)



Základní příkazy Secure Shellu:

Přihlášení ke vzdálenému počítači:

ssh john@drs.ipm.cz

Přenesení souboru z lokálního do vzdáleného počítače:

scp file.dat john@drs.ipm.cz:~/

Přenesení více souborů z lokálního do vzdáleného počítače:

scp file*.dat john@drs.ipm.cz:~/

Přenesení souboru ze vzdáleného do lokálního počítače:

scp john@drs.ipm.cz:~/file.dat .

Přenos souborů přes ssh pomocí GUI (Windows): **WinSCP**



awk je skriptovací jazyk, který umožňuje velmi efektivní dávkové zpracování souborů. Soubor se čte řádek po řádku a zpracovává interpreterem.

Jednoduchý příklad:

Datový soubor (xyz.dat):

0.0	11.2	1.6
0.2	14.1	12.4
0.4	21.7	16.4
0.6	43.1	12.1
0.8	22.1	8.9
1.0	11.5	0.1

awk: \$0 ... celý řádek
 \$1 ... první záznam
 \$2 ... druhý záznam
 ...

Výběr dat v prvním a třetím sloupci:

awk '{print \$1,\$3}' xyz.dat > xz.dat

Soubor xz.dat:

0.0	1.6
0.2	12.4
0.4	16.4
0.6	12.1
0.8	8.9
1.0	0.1

Pokročilé použití awku:

Struktura:

Tato část se provede **před začátkem** zpracování souboru:

```
BEGIN {  
}
```

Tato část se provádí po každém přečtení nového řádku, popř. za určitých předem daných podmínek:

```
{ ... }
```

Tato část se provede **po ukončení** zpracování souboru:

```
END {  
...  
}
```

```
#!/usr/bin/awk -f  
  
# This script is used to convert the data in file energy.dat (variation of the energy of the block  
# with the image number) to the dependence of the line energy of the dislocation on the  
# transformation coordinate, i.e. the Peierls barrier of the dislocation. If lastonly is true, it  
# only saves the Peierls barrier obtained from the last set of energies saved in the input file. The  
# output file contains two columns: column 1 = xi [A], column 2 = V [meV/A]. Here, xi is the  
# distance along a straight line connecting the two neighboring equivalent lattice sites in the slip  
# plane.  
  
BEGIN {  
    nimg = 32;  
    img = 0;  
    elem = "W";  
    latpar = 3.1652;  
    b = latpar*sqrt(3.0)/2.0;  
    a0 = latpar*sqrt(2.0/3.0);  
    lastonly = 1;  
    print sprintf("Processing the energies for element: %s", elem) > "/dev/tty";  
    print sprintf("Lattice parameter: %0.4f", latpar, " A") > "/dev/tty";  
    print sprintf("Burgers vector magnitude: %0.4f", b, " A") > "/dev/tty";  
    print sprintf("The site-to-site distance in the slip plane: %0.4f", a0, " A") > "/dev/tty";  
    if (lastonly) {  
        print "Saving only the Peierls barrier corresponding to the last iteration." > "/dev/tty";  
    } else {  
        print "Saving the Peierls barrier corresponding to all iterations in the input file." > "/dev/tty";  
    }  
}  
  
(img >= 0) {  
    if (NF != 0) {  
        xi = $1;  
        V = $2;  
        if (img == 0) {  
            V0 = V;  
        }  
        xi = xi/(nimg+1)*a0;  
        V -= V0;  
        V = V*1000.0/b;  
  
        if (!lastonly) {  
            print sprintf("%8.4f %8.4f", xi, V);  
        } else {  
            data[img,0] = xi;  
            data[img,1] = V;  
        }  
  
        if (img < nimg+1) {  
            img++;  
        } else {  
            img = 0;  
        }  
    } else {  
        if (!lastonly) {  
            print "";  
        }  
    }  
}  
  
END {  
    if (lastonly) {  
        for (img=0; img<=nimg+1; img++) {  
            xi = data[img,0];  
            V = data[img,1];  
            print sprintf("%8.4f %8.4f", xi, V);  
        }  
    }  
}
```

sed je skriptovací jazyk, který umožňuje jednoduché nahrazování textu v souboru jiným textem.

Jednoduchý příklad:

Datový soubor (dislo.tmp):

```
1
TUNGSTEN      C11: 0.5224E+01    C12: 0.2044E+01    C44: 0.1606E+01
X: -1 2 -1    Y: -1 0 1    Z: 1 1 1    B: 1 1 1    |B| : 0.8660
$xdislo $ydislo 0.0000
-0.2676259E-01 -0.9840635E+00
 0.1000000E-03  0.1031896E+01
 0.2676259E-01 -0.9840635E+00
 0.4020249E+00  0.1527066E-02 -0.4035520E+00
-0.2330429E+00  0.4650967E+00 -0.2320539E+00
-0.2365572E-03  0.4313241E-03 -0.2373886E-03
 0.4942613E+00  0.9867557E+00  0.4924945E+00
 0.8530366E+00 -0.3048607E-02 -0.8560852E+00
 0.2884192E+00 -0.2886777E+00  0.2889331E+00
```

sed 's/\$xdislo/0.0000/; s/\$ydislo/0.4714/' dislo.tmp > dislo.dat

Výstup (dislo.dat):

```
1
TUNGSTEN      C11: 0.5224E+01    C12: 0.2044E+01    C44: 0.1606E+01
X: -1 2 -1    Y: -1 0 1    Z: 1 1 1    B: 1 1 1    |B| : 0.8660
0.0000 0.4714 0.0000
-0.2676259E-01 -0.9840635E+00
 0.1000000E-03  0.1031896E+01
...
```




Operační systém vycházející ze standardu UNIX. První vydání r. 1991 (Linus Torvalds).

Jádro systému je vyvíjeno odděleně od aplikací.

Open Source – vývoj probíhá celosvětově ve skupinách zaměřených na jádro, grafiku, multimédia, ...

Mnoho distribucí

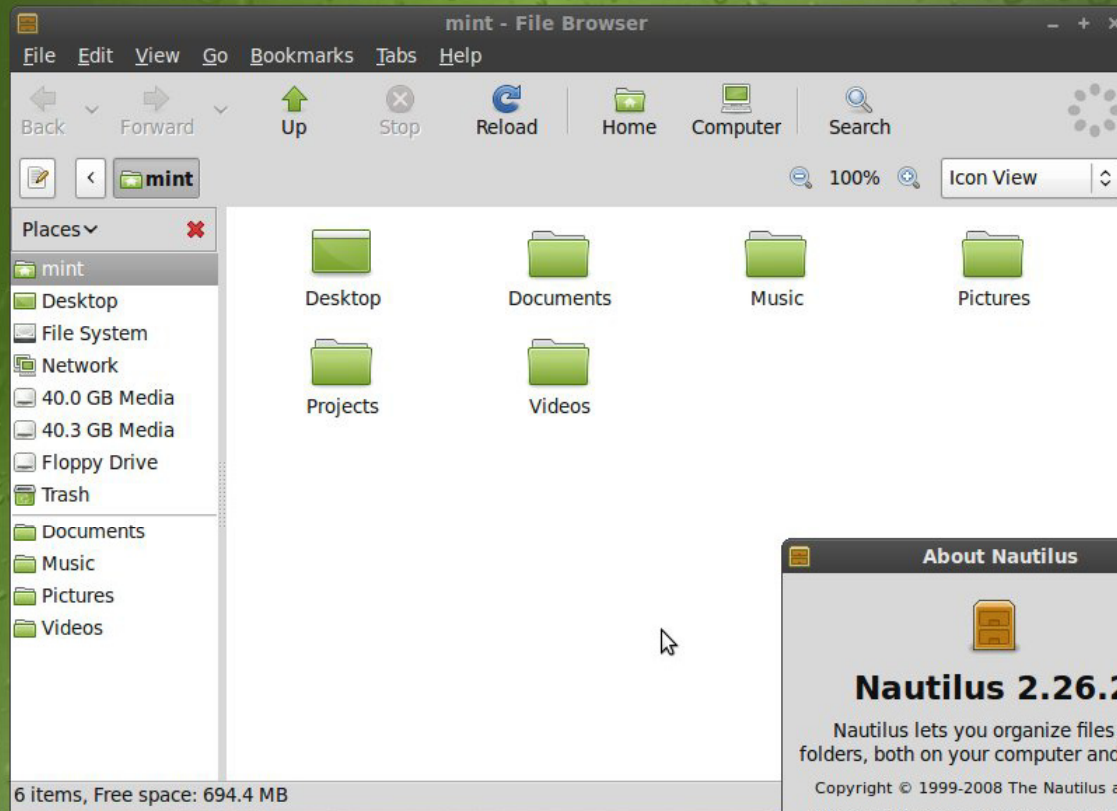
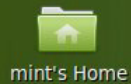
(viz. www.distrowatch.com):

NextSTEP (jádro Mac OS X) je v podstatě klon FreeBSD, což je jedna z variací UNIXu.

Page Hit Ranking		
Data span:		
Last 6 months Refresh		
Rank	Distribution	H.P.D*
1	Mint	3408▲
2	Mageia	2558▲
3	Ubuntu	1891▼
4	Fedora	1412▬
5	openSUSE	1329▼
6	Debian	1280▲
7	Arch	1217▲
8	PCLinuxOS	1035▲
9	Zorin	904▲
10	CentOS	815▲
11	Slackware	784▲
12	Puppy	784▲
13	Snowlinux	714▬
14	SolusOS	626▼
15	Lubuntu	605▼

a mnoho dalších ...

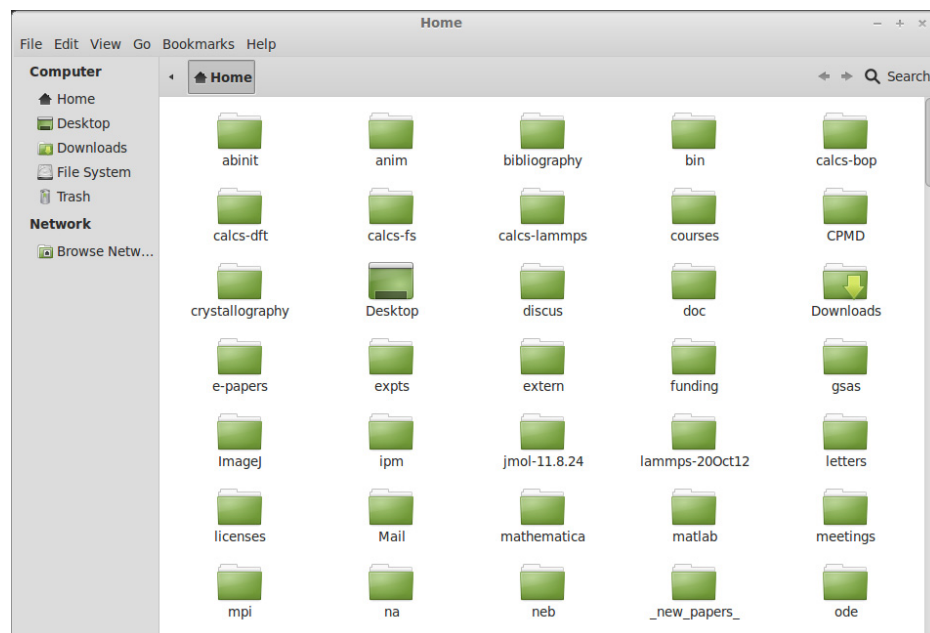
Pracovní plocha Linux Mint



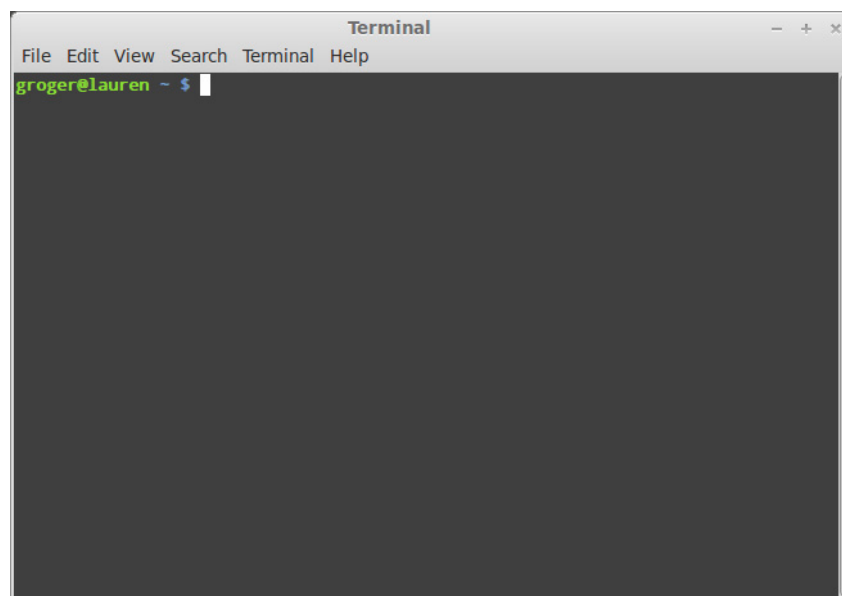
Software Manager



Window Manager



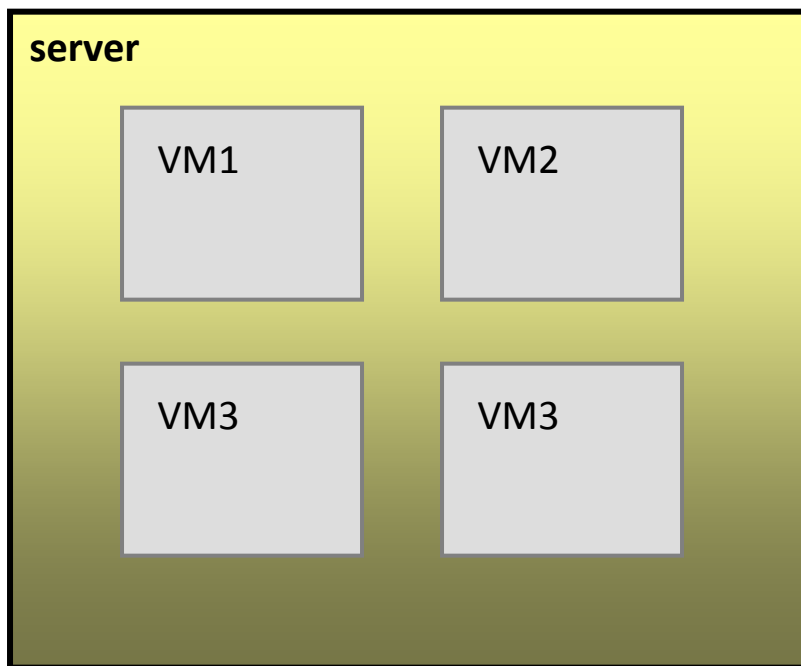
Terminal:



Virtuální stroje

Jedná se o **simulaci** stroje (počítače), který je zpravidla odlišný od toho, na kterém tato simulace běží. Např. potřebujeme-li aby jiný operační systém běžel jako program v jiném operačním systému.

Koncept:



VMWare Player (Windows, Mac, Linux)

www.vmware.com



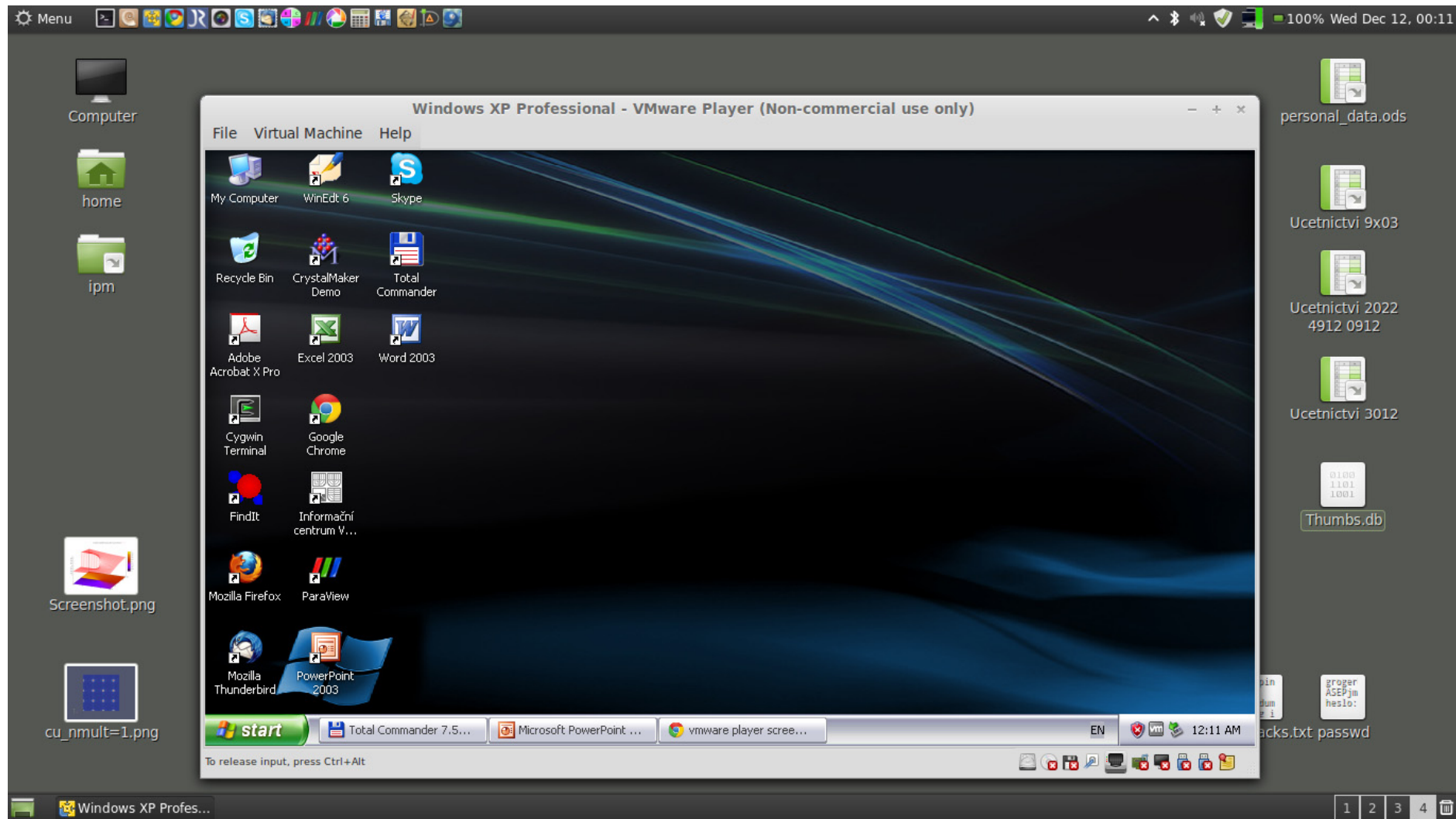
Pro nekomerční použití zdarma stáhnutelná implementace virtuálních strojů.

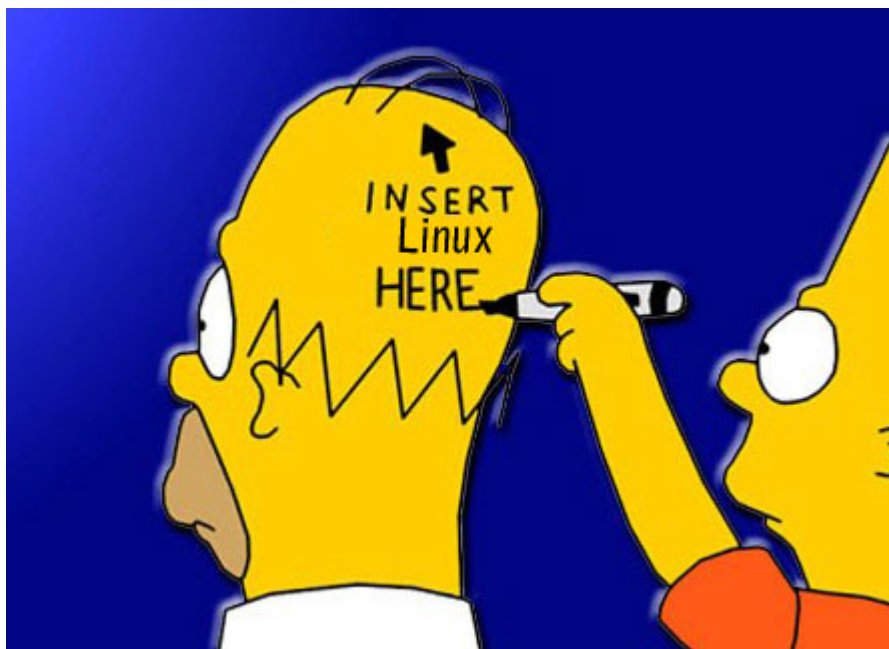
Umožňuje nainstalovat jakýkoliv OS pod jiným nebo stejným OS.

Část paměti je rezervována jako paměť virtuálního stroje. Sdílení harddisku, tiskáren, apod.



Windows XP běžící pod Linuxem:





... anebo do Windows přes **vmplayer**

Ke stažení na
<http://groger.ipm.cz>