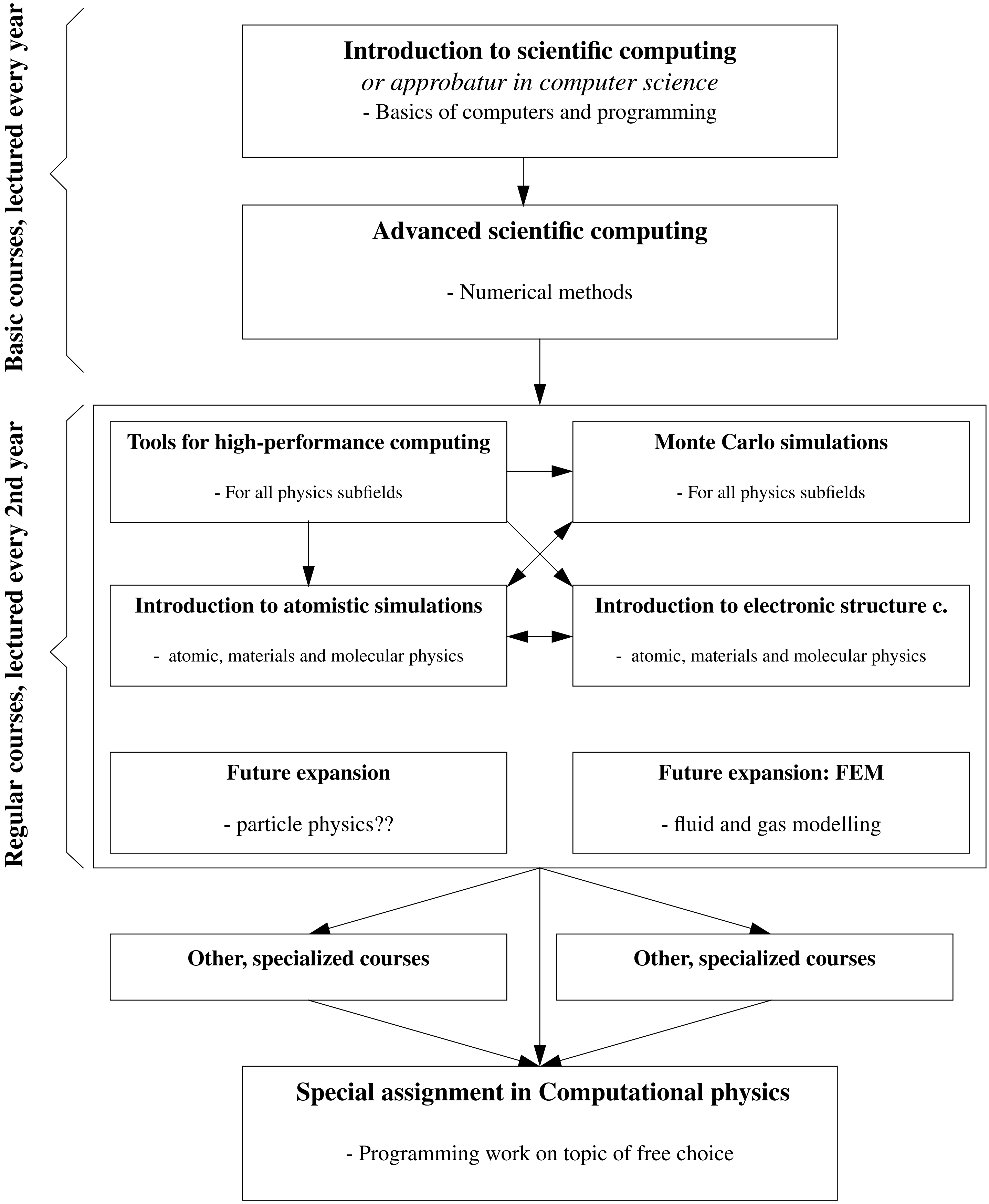
11.1 2003

Master plan for computational physics teaching at the University of Helsinki

http://www.physics.helsinki.fi/~fyl_www/suomi/laskfys/



53363-0 Introduction to atomistic simulations 2003

Lecturer: prof. Kai Nordlund (kai.nordlund@helsinki.fi, tel. 19150007)
Exercise assistant: the same, as it seems now.

Lecture: Tue 12-14 room
Lectures are given in Finnish when no foreigners are present
Exercises: Thu 12-14 room

- The idea of the course is to teach the students the basics of atom-level computer simulations, which are widely used in materials and atomic physics, chemistry and biology.

- The course deals with 4 basic simulation types: molecular dynamics (MD), Metropolis Monte Carlo (MMC), conjugate gradients (CG) and genetic algorithms (GA)
    - During the first part of the course a basic MD code is written under guidance in several steps during the exercises
    - After this the MD code is used in applications (this is the fun part!)
    - The ambitious students perhaps get to write an MMC code

Course evaluation:

- exercises 50 % of the points, plus possible bonus exercise points
- exam 50 %
- 45 % of the points: 1-/3
- 89 % of the points: 3/3

Exercises

The exercises are returned by email to the assistant no later than the Tuesday before the exercise. Many of the exercises involve writing subroutines or full computer programs. These will be compiled, and **if they do not compile, the exercise return automatically gives 0 points.**

The programs are to be returned either in Fortran90 or C.

- **Poll on language preference.**
- **Poll on Unix system access**

WWW-page of course: http://beam.helsinki.fi/~knordlun/atomistiset/

Contents

Literature

• **Lecture notes**

As background information you can use e.g.:

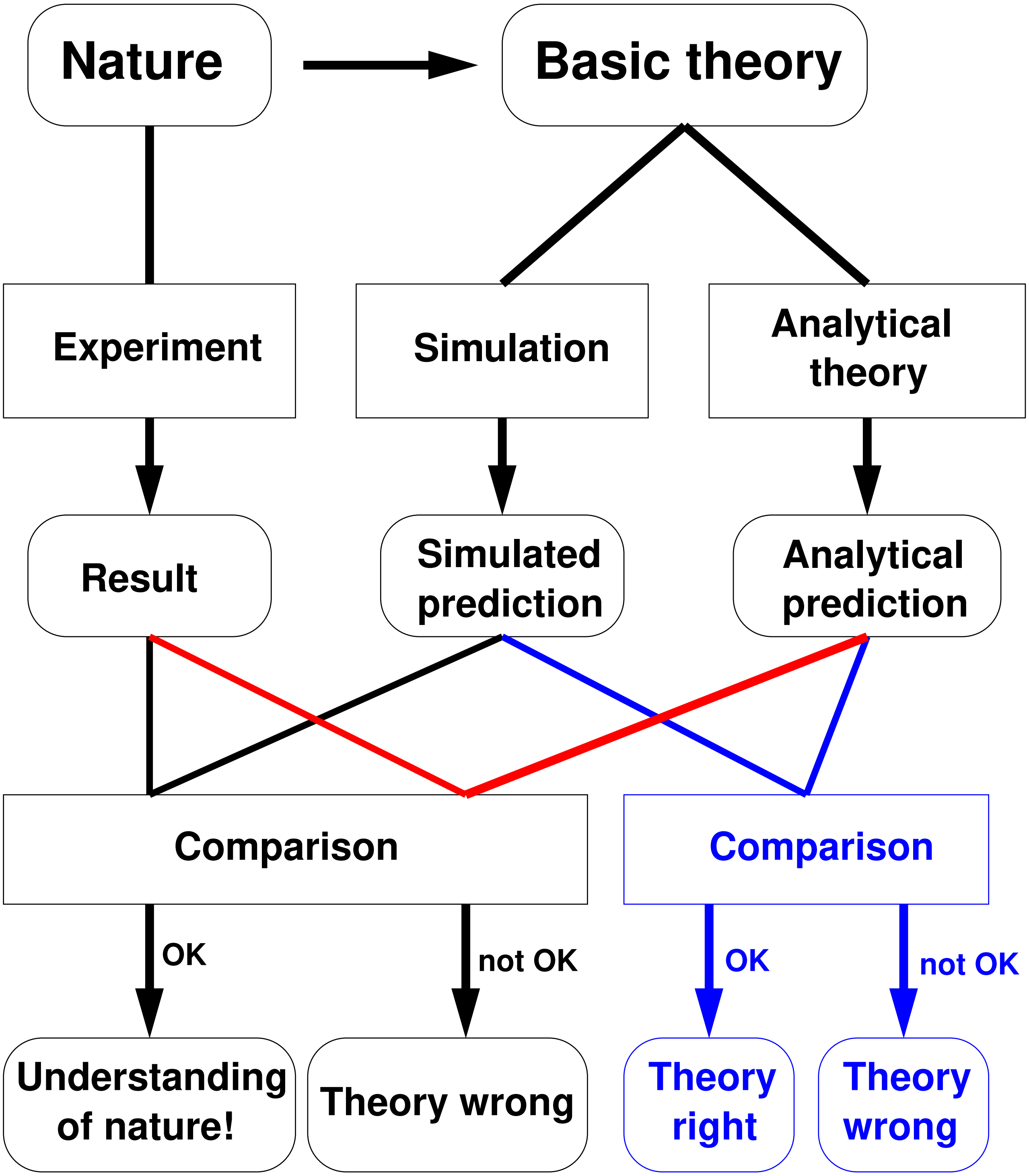
• Allen, Tildesley: "Computer simulation of Liquids" (Oxford University Press, Oxford, England, 1989)
• J. von Boehm: "Molekyylidynamiikka-menetelmä" (Otatieto, Espoo, 2000)

• The lecture notes will appear to the web a bit before the lecture.

• The notes of the previous courses (1999 and 2001) are in the web. But these are updated and corrected so it is better to wait for the new stuff.

• The web page also has links to similar courses elsewhere in the world

Computer simulations in physics



- Simulation can bridge the gap between theory and experiment
- Sometimes only choice (theory too complicated)
- Sometimes simulation impossible: not enough computer capacity
- Also comparison between analytical theory and simulation: if both are based on the same basic theory (e.g. Newtons laws), but analytical theory uses approximations, simulation can be a perfect way to test the approximation

Atomistic simulations: What is it?

• Model where the basic object is a (roughly) spherical object

• This object can be e.g. an

- Atom (surprise surprise!)
- Lattice defect
- Molecule
- Nanocluster
- A particle in a fluid

- (A planet or part of a galaxy)

• On this course, we almost always talk about "atoms", but in many cases the algorithms are such that the "atom" could be almost any of the above. **!**

• Application areas e.g.:

- Atom movement in equilibrium: thermodynamics
- Nonequilibrium situations: irradiation, material heat or pressure processing, phase transitions, nucleation
- Properties of lattice defects
- Nanostructures: $N_{atoms} \sim 10^4 - 10^8$: can be simulated!
- Interactions inside a molecule: vibration, rotation, protein folding
- Intermolecular interactions
- Chemical reactions

What is it not?

• Continuum modelling (e.g. Finite Element Modelling, FEM)
• Fixed lattice or grid model
  - although here the limit is sometimes hard to draw
• Particle physics
• Electronic structure calculation (for fixed positions of nuclei)
  - But el. struct. calc. often used as basis for atomistic simulation

• Since the basic object is an atom, and a computer memory is limited, atomistic simulations are always somehow size limited.
  - Hence usually simulating macroscopic (mm size and up) objects is usually out of the question

Important types of atomistic simulations

- **Molecular or lattice statics**

  - Find the equlibrium state (energy, shape) of an atomistic system based on some interaction model

- **Molecular dynamics (MD)**

  - Simulate the dynamic atom motion based on some interaction model

- **(Atomistic) Monte Carlo (MC)**

  - MC is in the broadest sense any simulation which uses random numbers
  - Even most MD simulations do use random numbers, but they are still conventionally not considered true MC simulations.

  - There are a few varieties of MC which are often used for atomistic simulations. The maybe most important are:

    - **Metropolis MC (MMC)**
      - Simulate a thermodynamic ensemble
      - Can also be used for energy minimization
    - **Kinetic MC**
      - Simulation of activated processes (e.g. migration)

  - The MC course deals with all this.
  - On this course MMC is briefly dealt with

- **Conjugate gradient (CG) - energy minimization**

  - An efficient way to find a local minimum
  - Can also be used for atoms

- **Genetic algorithms (GA)**

  - A (sometimes) efficient way to find a global minimum
  - Can also be used for atoms

- **Binary collision approximation (BCA)**
  - In nuclear and ion beam physics (and almost nowhere else)

How to present atomistic data

- **There exist about a zillion different file formats for presenting atom positions**
  - I will not even attempt a systematic overview.

Instead an example: how should we present the coordinates for 8 Cu atoms in the corners of the unit cube.

- Trivial format "x y z":

```
0.0 0.0 0.0
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 1.0
1.0 1.0 0.0
1.0 0.0 1.0
0.0 1.0 1.0
1.0 1.0 1.0
```

- Downside: All file has to be read in before we know how many atoms there are
- No information about time (for a dynamic system)

- Trivial format 2: "x y z t"

```
0.0 0.0 0.0 3.0
1.0 0.0 0.0 3.0
0.0 1.0 0.0 3.0
0.0 0.0 1.0 3.0
1.0 1.0 0.0 3.0
1.0 0.0 1.0 3.0
0.0 1.0 1.0 3.0
1.0 1.0 1.0 3.0
```

- Downside: All file has to be read in before we know how many atoms there are

- **XYZ-standardiformaatti:** “name x y z temperature”

  - First line has number of atoms at this time
  -. Second line is comment

```
 8
Molecule name or comment or whatever
Cu 0.0 0.0 0.0 320.0
Cu 1.0 0.0 0.0 310.0
Cu 0.0 1.0 0.0 305.0
Cu 0.0 0.0 1.0 280.0
Cu 1.0 1.0 0.0 290.0
Cu 1.0 0.0 1.0 320.0
Cu 0.0 1.0 1.0 310.0
Cu 1.0 1.0 1.0 320.0
```

- The fifth column can also hold other information, or be empty
- It is a very good idea to include useful information on the second line, e.g.

```
 8
Frame number 1 3.0 fs boxsize 3.0 3.0 3.0
Cu 0.0 0.0 0.0 320.0
Cu 1.0 0.0 0.0 310.0
...
```

- For dynamic information, the info for each time can simply be put after each other in the same file:

```
 2
Frame number 1 0.0 fs boxsize 3.0 3.0 3.0
Cu 0.0 0.0 0.0 320.0
Cu 1.0 0.0 0.0 310.0
 2
Frame number 1 2.0 fs boxsize 3.0 3.0 3.0
Cu 0.1 0.0 0.0 330.0
Cu 1.1 0.1 0.0 300.0
 2
Frame number 1 4.0 fs boxsize 3.0 3.0 3.0
Cu 0.2 0.1 0.0 340.0
Cu 1.2 0.1 0.0 290.0
...
```

Visualization of atomic data

- The simplest, most obvious and still very often the best way to visualize atomic data is to plot each atom as a sphere, either statically or dynamically

- Although this may not seem like very deep science, it is in practice extremely useful in many many cases, starting from debugging of a program, continuing to considering the structure of a molecule, finding new atomic structures and physical phenomena, and finally to making it to the cover of the journal Nature (the holy grail for basic science researchers).

- The other important thing to be able to do is plot bonds between atoms. This is naturally carried out with sticks or cylinders connecting atoms.
  - "Ball and stick"-model

- As with file formats, there are about a zillion programs which can do that.
  - I will not even attempt a systematic overview

- One much used visualization program is RasMol. It is

  + free and open source
  + works at least in Unix, VMS, Windows, OS/2 and Mac
  + well written code, easy to modify for your needs
  + supports many of the most common chemistry formats, including XYZ
  + can produce publication-quality output

  - poor at adding text to the graphics, has no font handling at all
  - can not draw much else than atoms, bonds and protein backbones

  • http://www.bernstein-plus-sons.com/software/rasmol/

  • I have installed rasmol to both the KuKa and main computer science Alpha Unixes in the directories /usr/local/contrib/bin/
    - Tested to work on Jan 12, 2003 in heavy.it.helsinki.fi and sirppi.helsinki.fi
    - To use it, either add /usr/local/contrib/bin/ to your Unix search path, or start with /usr/local/contrib/bin/rasmol

  • Should work under any X window system, or Windows with an X window emulator, when run from there

Practical advice on rasmol:

- In heavy.it.helsinki.fi

location: /usr/local/contrib/bin/rasmol
documentation: /usr/local/contrib/src/rasmol/RasMol26-301096/doc/manual.ps
whole package: /usr/local/contrib/src/rasmol/RasMol26-301096.tar.gz

To add /usr/local/contrib/bin/ to your search path do the following in your home directory in Unix:

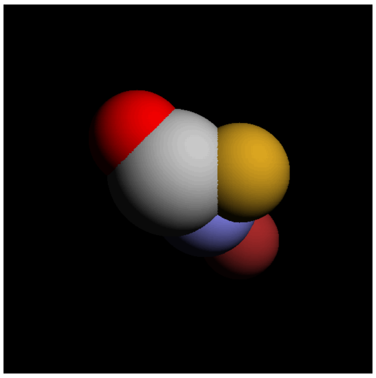
in .cshrc:

```
set path=($path /usr/local/contrib/bin)
```

and then start a new shell using `tcsh`

To test it, create e.g. the following file example.xyz:

```
5
Physically meaningless test data
C 0.0 0.0 0.0 1.0
Au 2.0 0.0 0.0 2.0
O -1.0 -1.0 0.0 3.0
N 1.0 1.0 1.0 4.0
Cu 2.0 2.0 2.0 5.0
```



rasmol -xyz example.xyz

This should open a separate RasMol-window and leave the terminal window with the RasMol command line interface with the prompt “Rasmol> “ . If you right away select from the “Display” mouse menu “Spacefill” the result should look like the figure to the right, in colors.

Test different RasMol window mouse menu options. You can rotate the molecule by holding down the left mouse button and moving the mouse pointer in the window. By holding down the right mouse button you can move the molecule.

For XYZ files rasmol calculates automatically bonding information between atoms, assuming the length unit is Ångströms and standard covalent radii, for a small enough number of atoms.

Some useful rasmol commands

Command line options, given by rasmol -h:

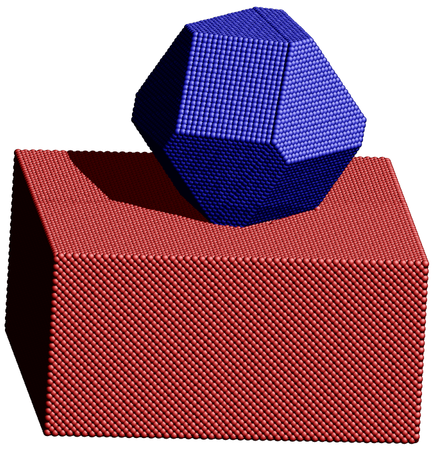
```
usage: rasmol [-knhacks] [-nodisplay] [-script scriptfile] [[-format] file]
    formats: -pdb -nmrpdb -mopac -mdl -mol2 -xyz -alchemy -charmm -direct*

-geometry x y : Set drawing area size
-knhacks*     : Use Kai Nordlunds horrifyingly ugly hacks
-kai*         : same as -knhacks
-noupper*     : Don't uppercase atom names
-xyzbonds*    : Enable bond definitions in XYZ files (KN)
-xyzanim tsleep* : Make xyz animation of file
-bondmax natoms* : Maximum number of atoms allowing bond search
```

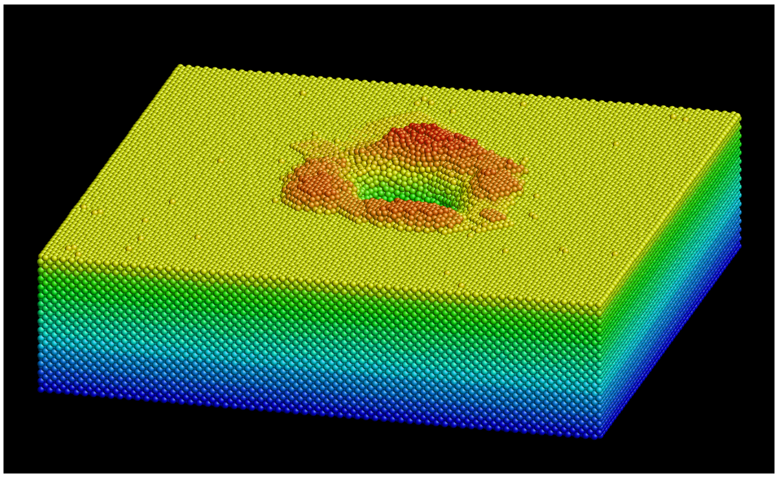
* Nonstandard option by Kai Nordlund

Useful Rasmol> command line options (see also “Quick Reference Card”):

load xyz file	Read in a file
write gif image.gif	Stora an image in the gif format
write ppm image.ppm	Store an image in the ppm format
write ps image.ps	Store an image in the ps format
zap	Remove all data, needed before new load command
quit	
wireframe <on/off/value>	Adjust bond width
spacefill <on/off/value>	Adjust atom size
spacefill temperature	Get atom size from column 5 in XYZ file
zoom 150	zoom, 100 = default size
set ambient <value>	Ambient light strength
set specular on	Use a nice 3D shade on atoms
set specpower <value>	Remove the 3D shade
set shadows on/off	Use/do not use atom shadowing

• A couple of examples of nice rasmol images





“Quick and dirty”-animations: dpc

- A simple way to make animations is to use Kai Nordlunds software dpc, or Jonas Frantz’s related gpdc

- dpc is available in the same places as rasmol.

  Basic usage for XYZ files: dpc xyz erase sort 2 3 4 5 moviefile.xyz

  “2 3 4” tells that the x, y- and z- info is taken from columns 2, 3 and 4.

  “5” does not mean anything for XYZ, but must still be there.

  All options are between “dpc” and “2 3 4 5”

- The program is not as flexible as rasmol, but it is very fast (it is written under plain Xlib, so all the complex graphics in higher-level packages does not slow it down)

- Help is given by command “dpc” with no options or “man dpc”

  Most important options

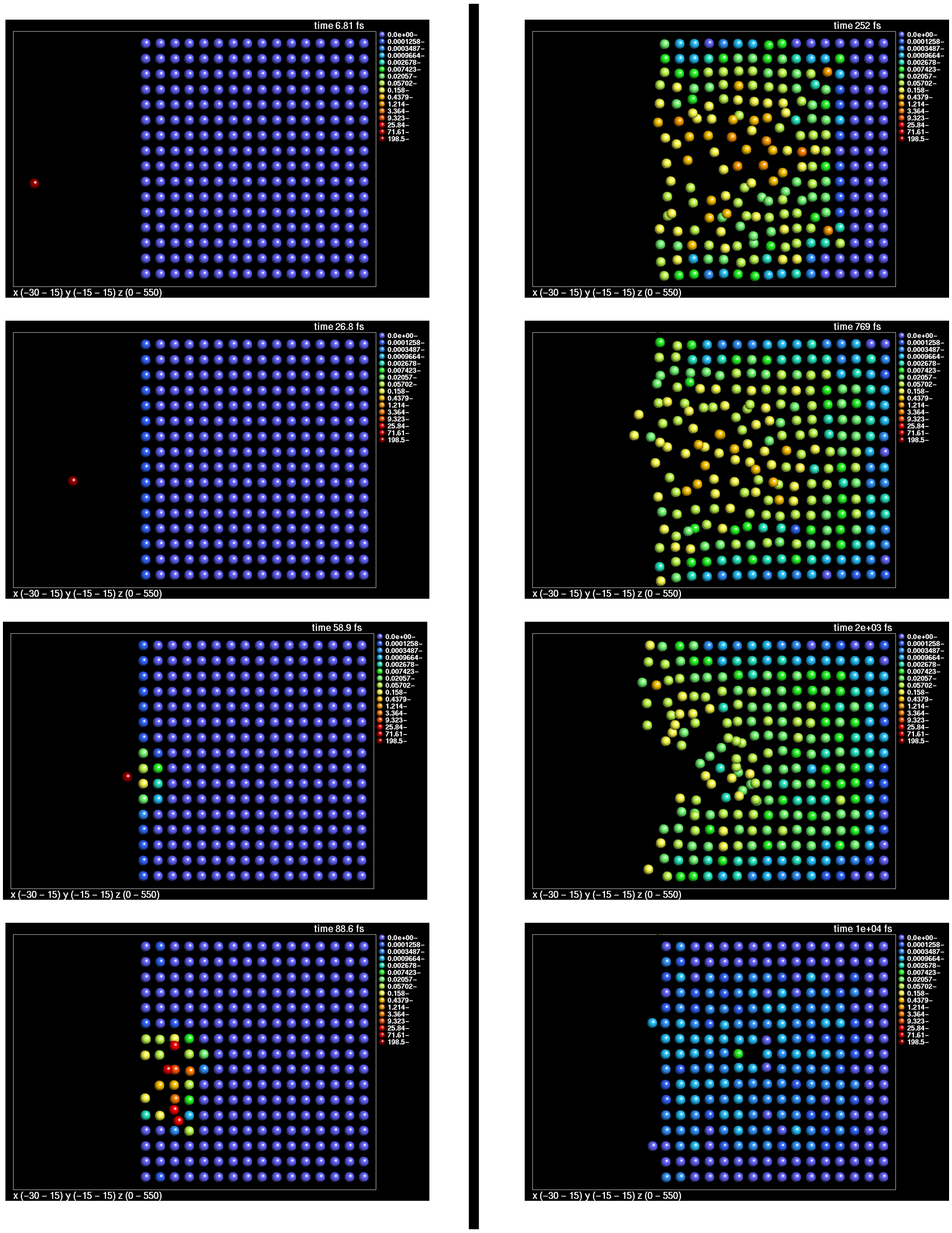
```
s 600 800          window size
sd 600 600         Draw area size
x 0 83             x limits
y 0 65             y limits
z 37.8 43.6        color (z) limits

m 1                form of atoms: 0 rect, 1-4 circle
d 4                dot size

gifdump            make gif file dump of each window frame

Example in heavy or sirppi (all should be on same command line):

dpc l m 4 d 20 s 800 600 y -15 15 x -30 15 z 0 550 xyz erase sort
4 2 6 5 /usr/local/contrib/src/dpc/slice.movie
```

- Source is available in /usr/local/contrib/src/dpc/

Example

- impact of 500 eV Au on Cu:

(Red spheres: energetic atoms, blue spheres cold)



- More animations (aplenty) below my web page

Making presentation animations

To make animations for the web or a (Powerpoint-like) presentation:

1. Use rasmol or dpc to make a separate gif image of every single time step
   - This can be made automatic in rasmol with the script features
   - In dpc with gifdump option

2. To make a gif animation for a web page, use
   /usr/local/contrib/bin/gifmerge

   - The program is quite easy to use, gifmerge -h :

```
Usage:
gifmerge [-<r>,<g>,<b>] [-<delay>] [-l<loops>] [-d<disp>] *.gif > anim.gif

   -<r>,<g>,<b>   set transparency, ie -192,192,192, default: no transparency
   -notransp       set transparency off (after you used -r,g,b before)
   -<delay>        set delay of between images in 1/100th secs, ie -100
                   default 50 (0.5secs)
   -l<loops>      set loop counter, ie -l0 (ever) or -l1000, default no loops
   -d<disposal>    set disposal 0 = no action, 1 = no dispose,
                                2 = restore background (default)
                                3 = restore previous
   -pos<x>,<y>     set offset position for image
   -nopos          reset offset position (default)

   or look at http://www.iis.ee.ethz.ch/~kiwi/GIFMerge/
```

   - So if you have e.g. images image01.gif - image99.gif:

```
gifmerge -l0 -25 image??.gif  > animation.gif
```

3. To make mpeg animations you can use e.g. ppmtompeg from the free ppm program package in Unix

4. To make AVI animations for Windows/Powerpoint you have to find some commercial software for the purpose, e.g. MainActor mave

A common practical problem in this is that many animation programs, e.g. rasmol, scales the plotting region from the outermost atoms. If the outermost atoms move a lot in a dynamic simulation, this leads to funny looking jumping of the atoms. A simple trick to circumvent this is to put in extra dummy atoms somewhat outside all the real ones at the same position for all time step. Then in the plotting just zoom in a bit to leave the dummy atoms out from the drawing region.