Nestlé
Good Food, Good Life

ESPResSo
Expansions, **S**ustainment, **PR**ogr**es**s and **S**o **o**n

Hanjo's view

1st Frankfurt Meeting on ESPResSo

14.07.2006

I apologize…

- … this will be the most ‘unfancy’ power point presentation you have ever seen.

Status of Espresso

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- Most flexible MD program
- ~ 61 thousand lines of code
- ~ 200 files
- A big mess!!!

- There is a lot of work to do:
  - Both on the existing stuff as well as for new extensions

Some order

- Core
- Data Organization
- Physics
- Potentials
- Statistics
- Helpers
- Tcl-scripts

Core

- main
- communication (mpi)
- initialize
- config (debug, error_handling, version)

Data / Organization

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- cells
  - grid, ghosts
  - domain_decomposition, layered, nsquare
- interaction_data
- particle_data
- topology
- Input/Output:
  - blockfile, binary_file
  - imd, vmd_socket

Physics

- integrate (thermostat, forces, verlet)
- forces
- energy
- pressure

Potentials

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Bonded	Non-bonded	Long-range	Special
fene	lj, lj_cosx	p3m	constraints
harmonic	morse	elc	molforces
rattle	soft_sphere	mmm_xd	comfix
subt_lj	buckingham	mmm_common	comforce
angle	gb	ewald	
dihedral	debye_hueckel	lb	
tab	tab	Maggs	

Statistics / Analysis

- statistics
- statistics_chain
- statistics_molecule
- statistics_cluster
- modes

Helpers

- bin
- fft
- parser
- polymer
- polynom
- random
- specfunc
- tuning
- utils
- uwerr

Tcl-scripts

- ABHmath
- auxiliary
- blockfile_support
- bundle
- convertDeserno
- countBonds
- init
- pdb
- polymer
- statistics

My-clean-up-the-mess-list

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- File names (long names, order (e.g. utils_fft),…)
- Kick out useless files from main directory
- Redistribution of file responsibilities
- Documentation
- List features that are not thoroughly tested.

File mess

- Kick out all script files from main directory
- As well as the helpers for configure
- blockfile_test.c ??

- Make a common beginning for files belonging to the categories:
  - statistics
  - helpers
  - potentials

- Do not use abbriviations like: gb, lb, lj, …
  - (as far as I remember we agreed on long file and variable names)

Documentation mess

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- No (or almost no) documentation
  - bin
  - comfix/comforce
  - config.c
  - integrate
  - maggs
  - modes
  - parser
  - polymer
  - random
  - rattle
  - softsphere
  - topology
- Needs update:
  - fft, grid, stand alone documentations

Stand Alone Documentation

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- We have to go through that and make a detailed plan what we would like to have here.

- What about the new users? What is missing? What is useful?
- Corrections by the ‘old guys’

Extensions that I miss

- For atomistic simulations
  - Important for coarse graining and bio stuff
  - Scripts for input of force fields and topologies
  - Pressure correction
  - Constraint algorithm for angular potentials
  - Test cases for atomistic simulations (water, a small protein, bilayer)
- Free energy calculations

Future items

- Polarizable Force Fields
- Still Monte Carlo