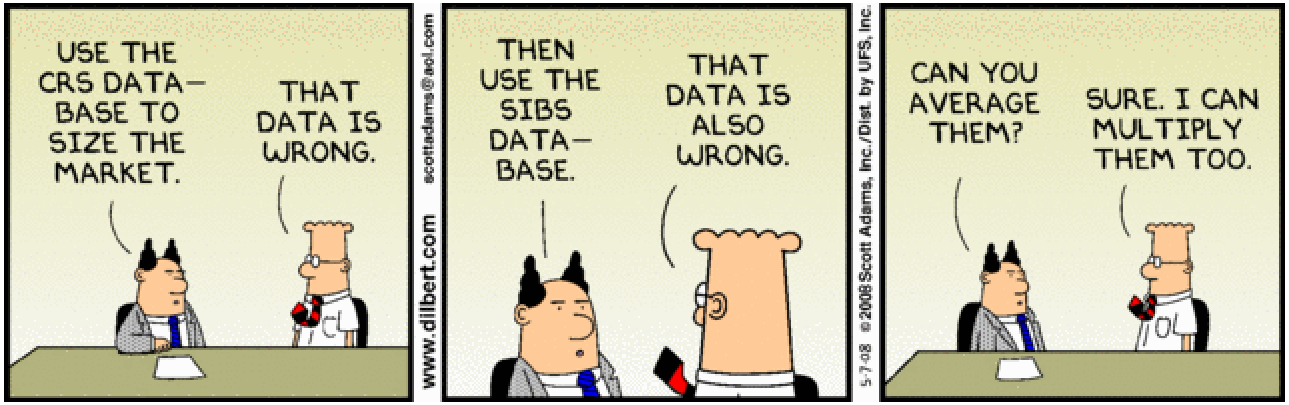
Hands-on: Data analysis and advanced scripting


USE THE CRS DATA-BASE TO SIZE THE MARKET.
THAT DATA IS WRONG.
scottadams@aol.com
www.dilbert.com
THEN USE THE SIBS DATA-BASE.
THAT DATA IS ALSO WRONG.
5-7-08 ©2008 Scott Adams, Inc./Dist. by UFS, Inc.
CAN YOU AVERAGE THEM?
SURE. I CAN MULTIPLY THEM TOO.

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Learning objectives

- "On-the-fly" analysis: use LAMMPS to compute/accumulate/average properties of interest while the simulation is running
  - Use "variable" commands to perform simple calculations
  - Use "compute" and "fix" commands for more elaborate calculations
- Post-processing: use external tools (Python scripts) to perform additional analysis at the end of the simulation

This hands-on activity was derived from actual research work (see paper in *reference* folder)

Bulk water – basic simulation

- Enter directory *simulation-bulk/1*
- Inspect input files: in.bulk, forcefield.TIP3P, data.singleTIP3P
- Run: $ lammps < in.bulk
- Inspect output
- Visualize:
  - – Directly (.jpg, .mpg)
  - – With VMD (.lammpstrj)

  Pregenerated visuals available in *viz* subdirectory

Bulk water – potential energy

- Work in directory 1/
- Task: modify input script to compute and output the potential energy per molecule in units of kcal/mol
- Hints:
  - Check out “compute pe” command
  - Remember to normalize by the number of molecules
- Result should be ~ -9.9 kcal/mol
- When finished, compare your script and results with content of directory 2/

Bulk water – mass density

- Work in directory 2/
- Task: modify input script to compute and output the system density in units of g/cm^3
- Hints:
  - Use *variable* commands:
    - To define useful constants (molecular mass, Avogadro's number, conversion factors, etc.)
    - To perform the actual calculation
- Result should be ~ 1 g/cm^3
- When finished, compare your script and results with content of directory 3/

Bulk water – radial distribution function (RDF)

- Work in directory 3/
- Task: modify input script to compute and output the oxygen-oxygen RDF
- Hints:
  - Use *compute rdf*
  - Obtain oxygen type from data file
  - Use fix ave/time to generate output file
- When finished, compare your script and results with content of directory 4/

Bulk water – radial distribution function (RDF) post-processing

- Work in directory 4/
- Output gOO.rdf contains comments, extra data, cannot be plot directly
- File gOO.rdf needs to be post-processed
- Check out analysis-tools/rdf2data.py (open with text editor and see comments for usage instructions)
- Example:

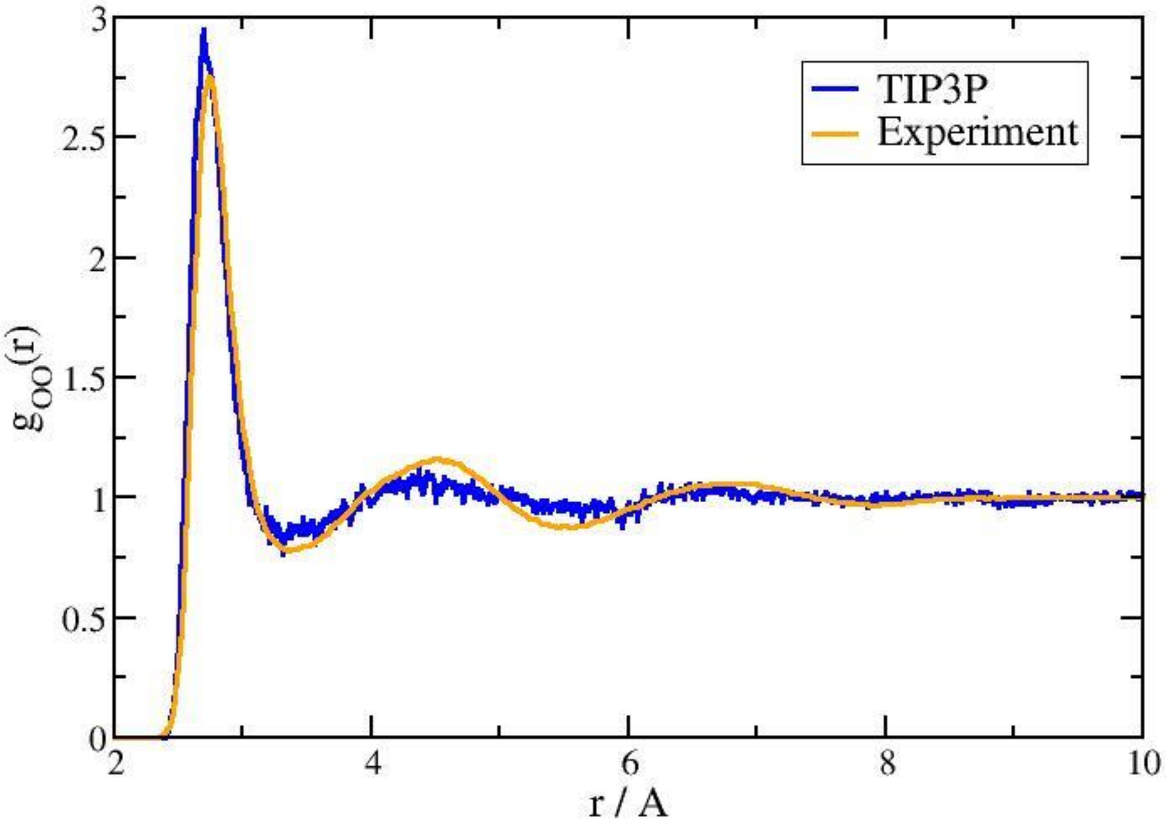
```
$ python ../../analysis-tools/rdf2data.py gOO.rdf > gOO.dat
```

- gOO.dat is now 2-column matrix (r|gOO) which can be plotted together with reference experimental data:

```
$ xmgrace gOO.dat ../../reference/gOO-exp.dat
```

- Compare results with 4-post

RDF: simulation vs. experiment



Simulation curve is noisy because of short simulation time. For converged results, see paper in *reference* folder.

Bulk water – mean squared displacement (MSD)

- Work in directory 4
- Task: compute and output the MSD
- Hints:
  - Use *compute msd*
  - Assume oxygen MSD = water MSD
  - Use fix ave/time to generate output file
- When finished, compare your script and results with content of directory 5

Bulk water – Diffusion

- Work in directory 5
- Diffusion coefficient defined as:

$$D = MSD(t) / 6t$$

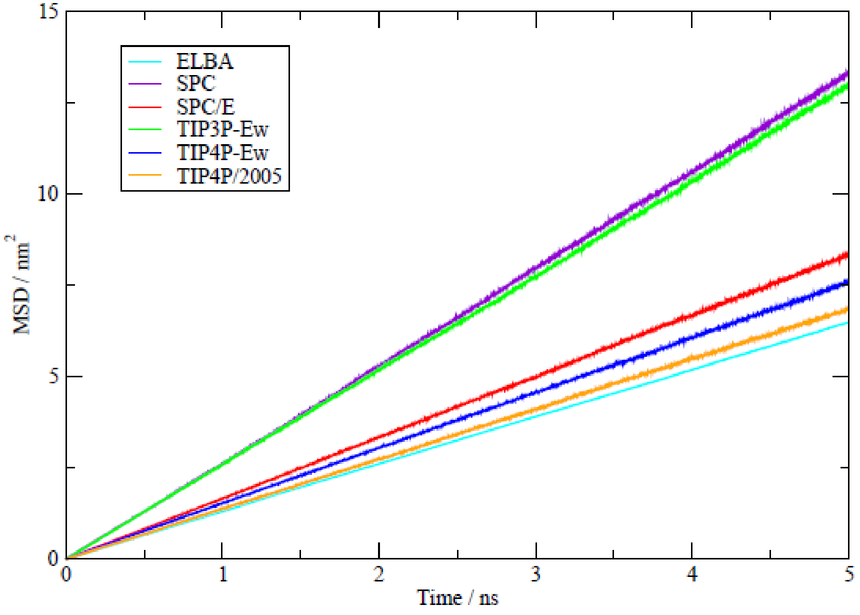
with t sufficiently large to get convergence

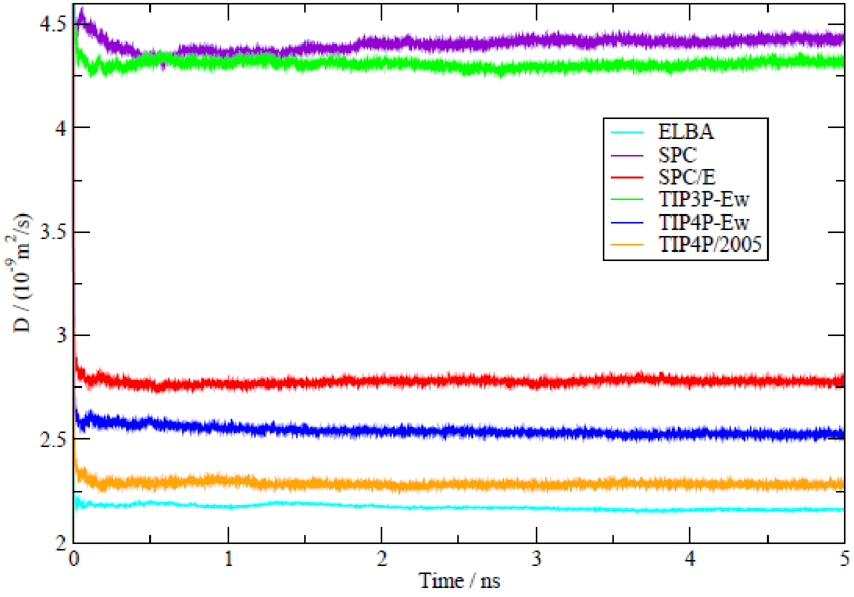
- MSD data can be post-processed to obtain D:
- Check out analysis-tools/msd2diff.py (open with text editor and see comments for usage instructions)
- Example:

```
$ python ../../analysis-tools/msd2diff.py wat.msd 2 3 > wat.diff
```

- Compare with 5-post

MSD and diffusion





Converged results from paper in *reference* folder

Water/vapor interface – basic simulation

- Enter directory *simulation-interface/1*
- Inspect input script
- Notice how the change_box command is used to increase z dimension and create water layers separated by vacuum layers
- Run: $ lammps < in.liquid-vapor
- Inspect output
- Visualize:
  - Directly (.jpg, .mpg)
  - With VMD (.lammpstrj)

  Pregenerated visuals available in *viz* subdirectory

Water surface tension

- Work in directory 1/
- Task: modify input script to compute and output the surface tension of the water-vacuum system in units of mN/m (milliNewton/meter)
- Surface tension = Lz * [Pz - (Px + Py) / 2] / 2
- Hints:
  - Use equal-style variables
  - Average with fix ave/time
  - Define conversion factors between LAMMPS units and required output units
- When finished, compare your script and results with content of directory 2/

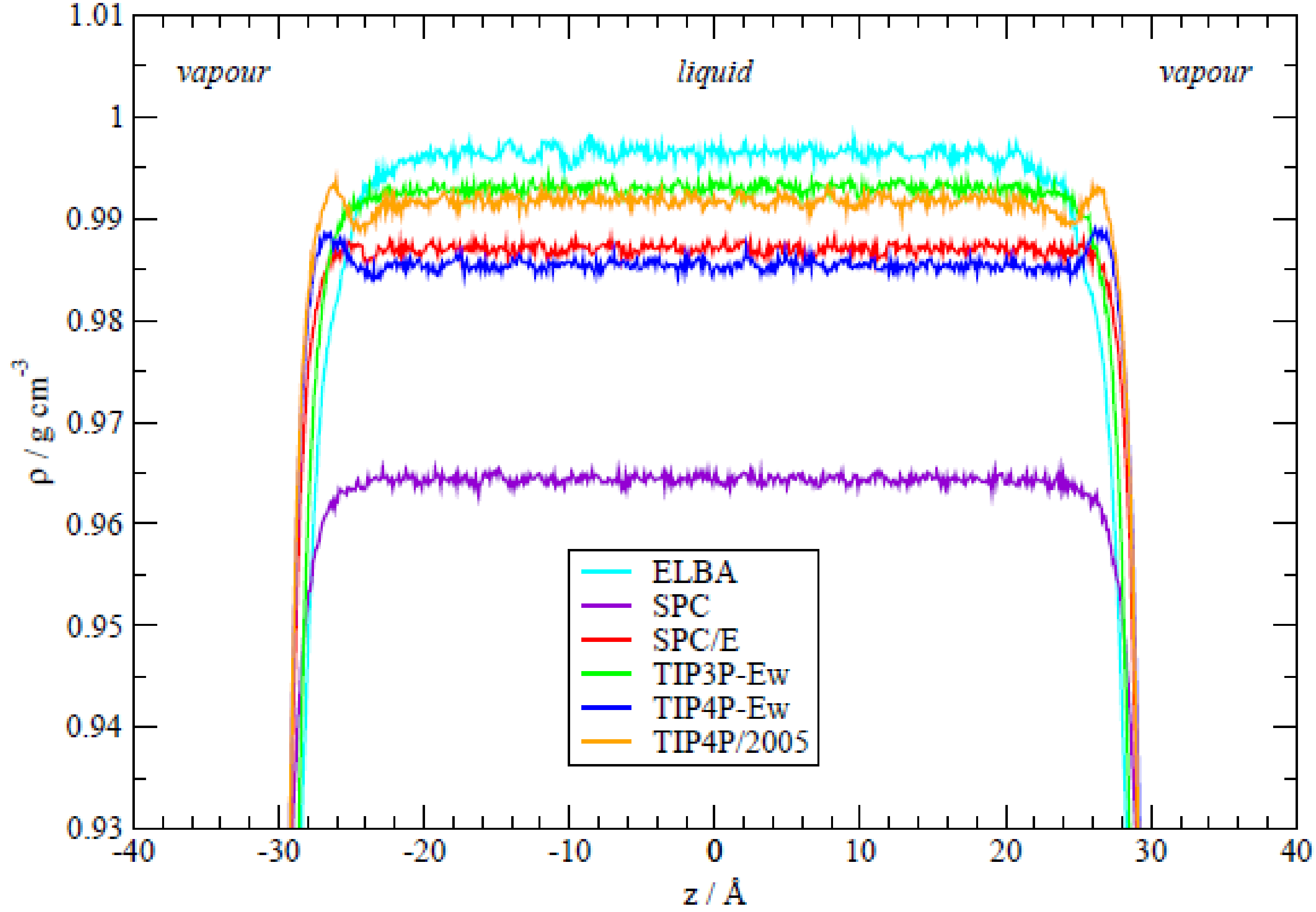
Water number density profile

- Work in directory 2/
- Task: modify input script to compute and output the number density profile across the water-vacuum interface
- Hints:
  - Use *fix ave/spatial* with appropriate keywords
  - Compute individual profiles for H and O
- When finished, compare your script and results with content of directory 3/

Water mass density profile

- Work in directory 3/
- Task: post-process H and O number density profiles to obtain total H_2O mass density profile
- Hints:
  - Use *../../analysis-tools/numDens2massDens.py* (open file with text editor and see comments about usage)
  - Compute individual profiles for H and O
  - To get total profile, see *../../analysis-tools/sumProfile.py*
- When finished, compare your results with content of directory 3-post/

Mass density profile across water-vapor interface for various models



Converged results (see paper in *reference* folder)