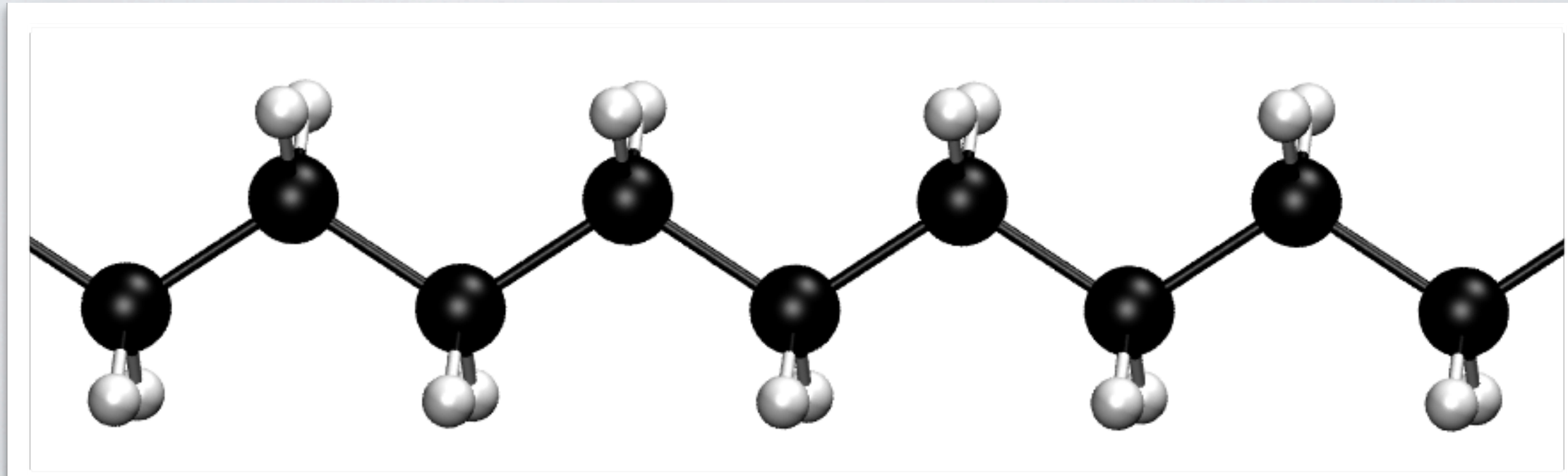
EXERCISE 6:

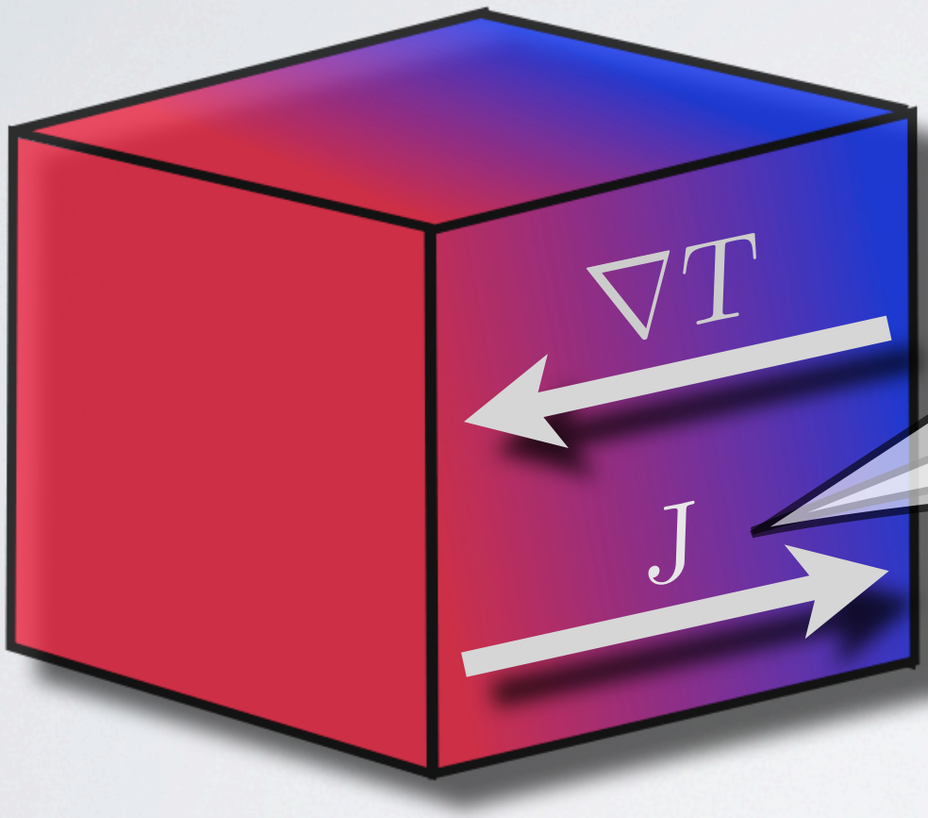
HEAT CONDUCTION OF A ONE-DIMENSIONAL CH_2-CHAIN



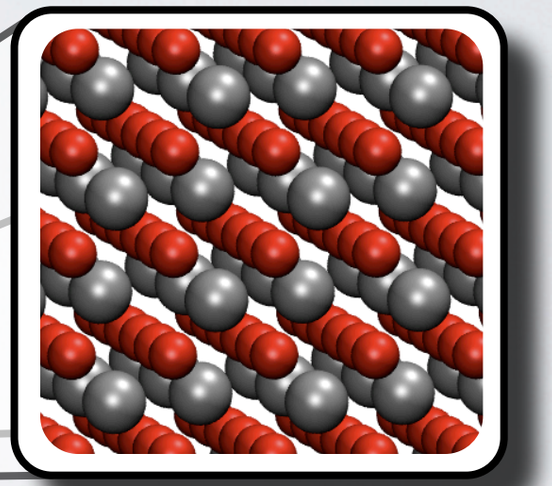
I. Introductory Talk

HEAT CONDUCTION

Macroscopic Effect:



Microscopic Nature:



$$\frac{\partial T(x,t)}{\partial t} - \alpha \frac{\partial^2 T(x,t)}{\partial x^2} = 0$$

Heat diffusivity

Can we calculate and understand the **heat diffusivity** from **first principles**?

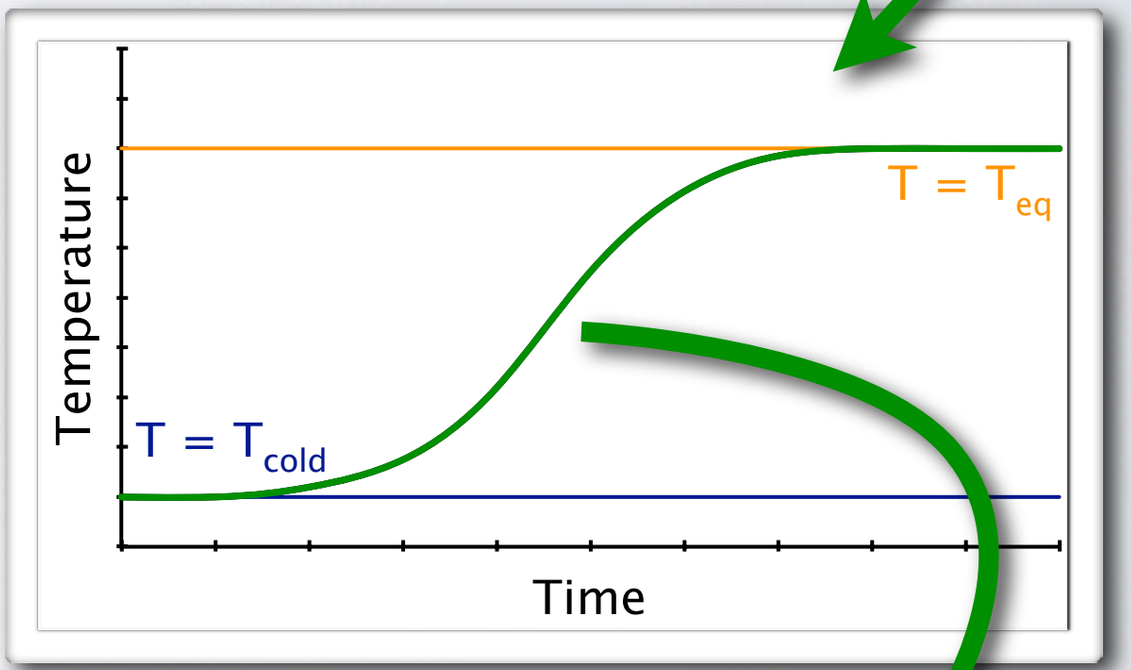
„LASER FLASH“ MEASUREMENTS

W. J. Parker *et al., J. Appl. Phys.* **32**,1679 (1961).

heat diffusion

$T = T_{hot}$

$T = T_{cold}$



Heat Diffusion Equation:

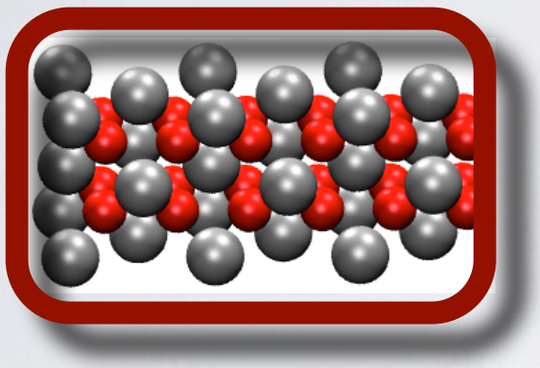
$$\frac{\partial T(x,t)}{\partial t} + \alpha \frac{\partial^2 T(x,t)}{\partial x^2} = 0$$

Extract the ***heat diffusivity α*** by fitting **T(x,t)**

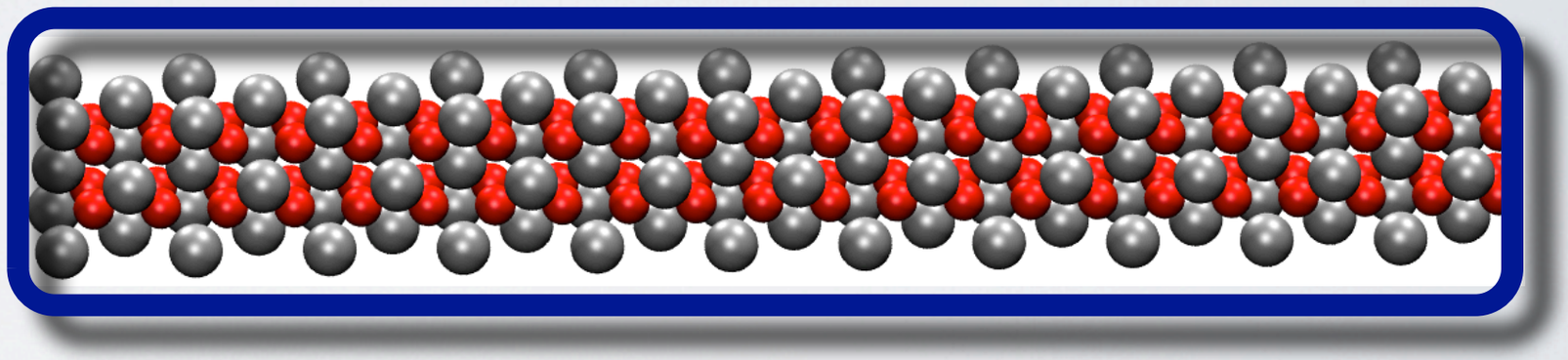
„LASER FLASH“ SIMULATIONS

T. M. Gibbons and S. K. Estreicher, *Phys. Rev. Lett.* **102**, 255502 (2009).

Mimic the ***„Laser-Flash Measurements“*** in ***ab initio MD simulations***:



hot SC



cold supercell

(A) Prepare two supercells: a small hot one and a large cold one.

(A) NON-EQUILIBRIUM PREPARATION

S. K. Estreicher, and T. M. Gibbons, *Physica B* **404**, 4509 (2009).

In the **quasi-harmonic approximation**, the **positions r_i** and the **velocities v_i** are related to the **vibrational eigenfrequencies ω_s** and -vectors **e_s**.

$$r_{0i} + \Delta\mathbf{r}_i = + \sum_s A_s(T) \frac{\cos(\Phi_s + \omega_s t)}{\sqrt{M_i}} \cdot \mathbf{e}_s$$

$$\mathbf{v}_i = - \sum_s A_s(T) \frac{\sin(\Phi_s + \omega_s t)}{\sqrt{M_i}} \cdot \omega_s \cdot \mathbf{e}_s$$

Maxwell-Boltzmann distributed amplitudes

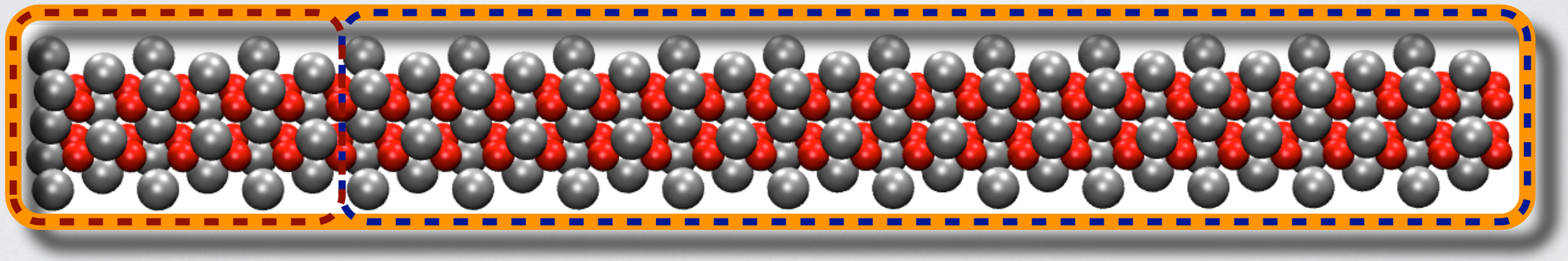
random phase

harmonic approximation

„LASER FLASH“ SIMULATIONS

T. M. Gibbons and S. K. Estreicher, *Phys. Rev. Lett.* **102**, 255502 (2009).

Mimic the ***„Laser-Flash Measurements“*** in ***ab initio MD simulations***:



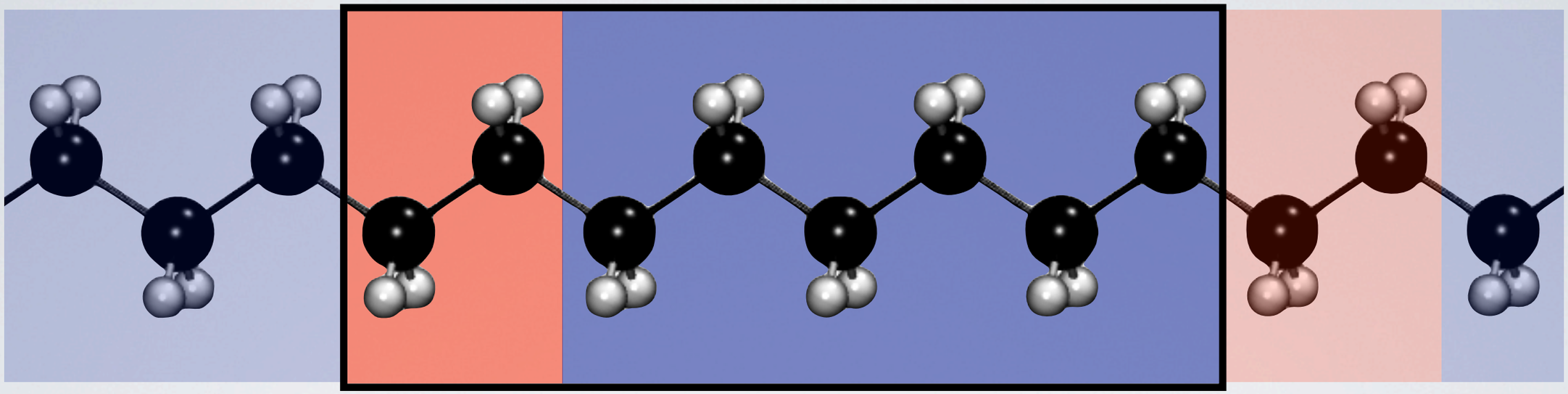
heat diffusion

(A) **Prepare two supercells:** a **small hot** one and a **large cold** one.

(B) **Connect** the **two** supercells, let the **heat diffuse** via **MD** and **monitor** the temperature profile **T(x,t)**.

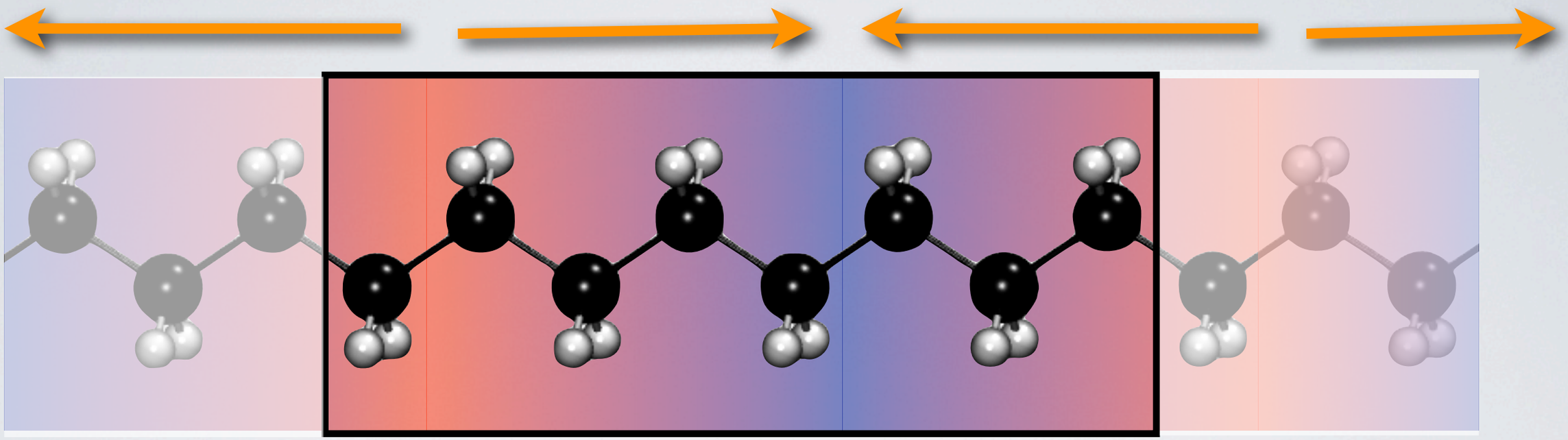
II. Application to $(CD_2)_8$

One-Dimensional CD_2-Chain



(A) Prepare two segments:
A **small hot one (C_2D_4)** and a **large cold one (C_2D_4)**.

One-Dimensional CD_2-Chain



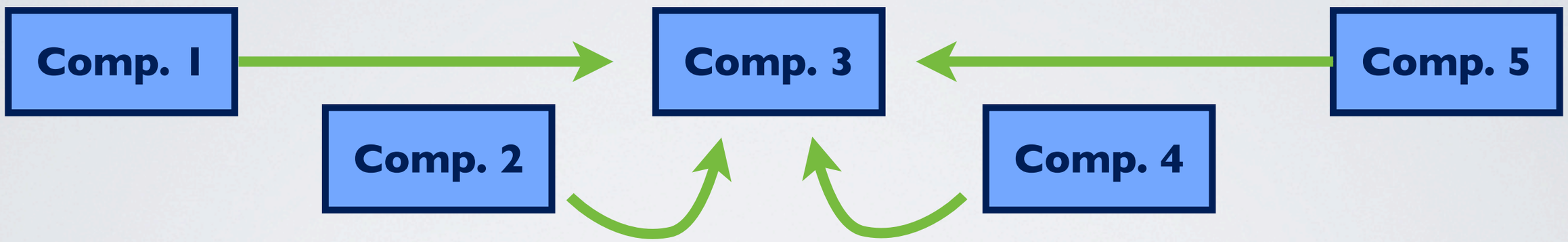
(A) Prepare two segments:
A **small hot one (C_2D_4)** and a **large cold one (C_2D_4)**.

(B) Monitor heat diffusion via *Ab Initio Molecular Dynamics*

This will be an overnight simulation!

One-Dimensional CD_2-Chain

Tomorrow Afternoon

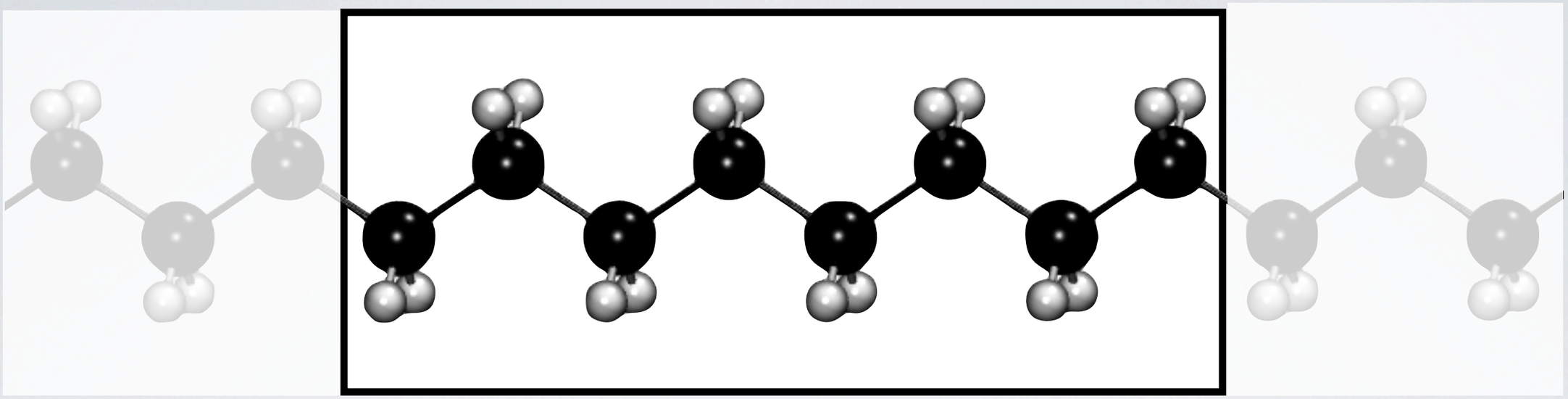


(A) **Each of you** will evaluate its **own trajectory.**

(B) **Each of you** will evaluate **all other trajectories.**

You will find all other trajectories in
`$HOME/tutorial5/exercise6`

One-Dimensional CD_2-Chain



The files

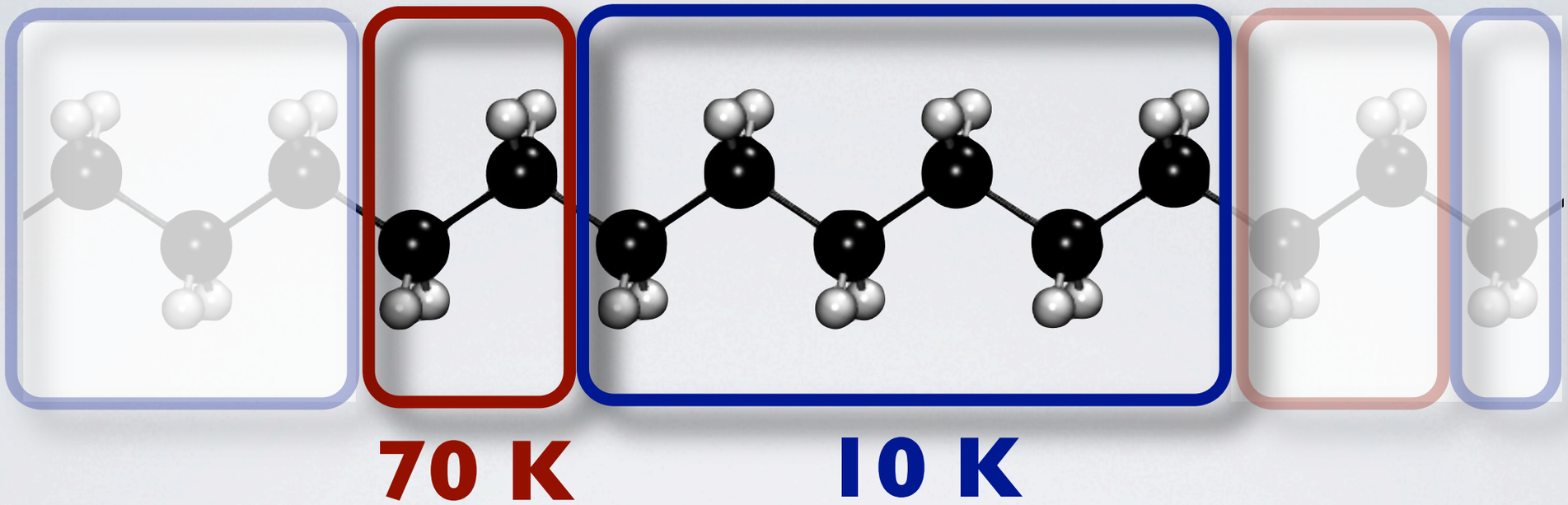
geometry.in ; control.in ; eigenfreq-and-vectors.dat

can be found in the directory

/pub/tutorial5/exercise_6

For the success of this exercise, it is essential that you use the provided input files!

Setup of the cell in non-equilibrium



File **control.in**:

```
#Generate non-equilibrium supercell
MD_QH_init      1     6      70.0     eigenfreq-and-vectors.dat
MD_QH_init      7     24     10.0     eigenfreq-and-vectors.dat
```

Index-range of atoms to which **this** line applies

Target-temperature for the selected **range** of atoms

ASCII-File containing the **eigenfrequencies** and **eigenvectors**

File **eigenfreq-and-vectors.dat** – Part I

 # Equilibrium geometry

lattice_vector	50.0	0.0	0.0		
lattice_vector	0.0	50.0	0.0		
lattice_vector	0.0	0.0	10.1017554400		
atom	0.0000000000	0.0000000000	0.0000000000	C	1
atom	0.6713400000	0.8823000000	0.0000000000	H	2
atom	0.6713400000	49.1177000000	0.0000000000	H	3
[...]	[...]	[...]	[...]	[...]	[...]
atom	49.1752312100	0.0000000000	8.8390360100	C	22
atom	48.5041200000	0.8823000000	8.8390360100	H	23
atom	48.5041200000	49.1176200000	8.8390360100	H	24

N.B. – Each atom has an **index**!

File **eigenfreq-and-vectors.dat** – Part II

 # Number of acoustic modes

n_acoustic	4

 # Eigenfrequencies at Gamma in meV (ascending order)

frequency	0.0000000000	1
frequency	0.0000000000	2
frequency	0.0000000000	3
frequency	0.0000000000	4
frequency	8.2962255208	5
frequency	8.2962255208	6
[...]	[...]	[...]
frequency	273.5062375662	72

Eigenfrequencies in ascending order

File **eigenfreq-and-vectors.dat** – Part III

 # Eigenvectors at Gamma (orthonormalized)
 # Mode 1 - Atoms 1 to 24 - Eigenfrequency 0.0000000000
[...]

 # Mode 5 - Atoms 1 to 24 - Eigenfrequency 8.2962255208

eigenvector	5	1	0.0	0.333450083948482	0.0
eigenvector	5	2	-0.027852301915242	0.157201713917909	-0.047378988713170
eigenvector	5	3	0.027852301915233	0.157201713917909	0.047378988713147
[...]	[...]	[...]	[...]	[...]	[...]
eigenvector	5	24	-0.006672545205799	0.037010655381660	0.083441653880655

 # Mode 6 - Atoms 1 to 24 - Eigenfrequency 8.2962255208
[...]

Eigenvectors for all modes

Start the *ab initio* MD run

PLEASE ENSURE THAT YOUR INPUT IS CORRECT:
For the success of this exercise, it is essential
that you use the provided input files!

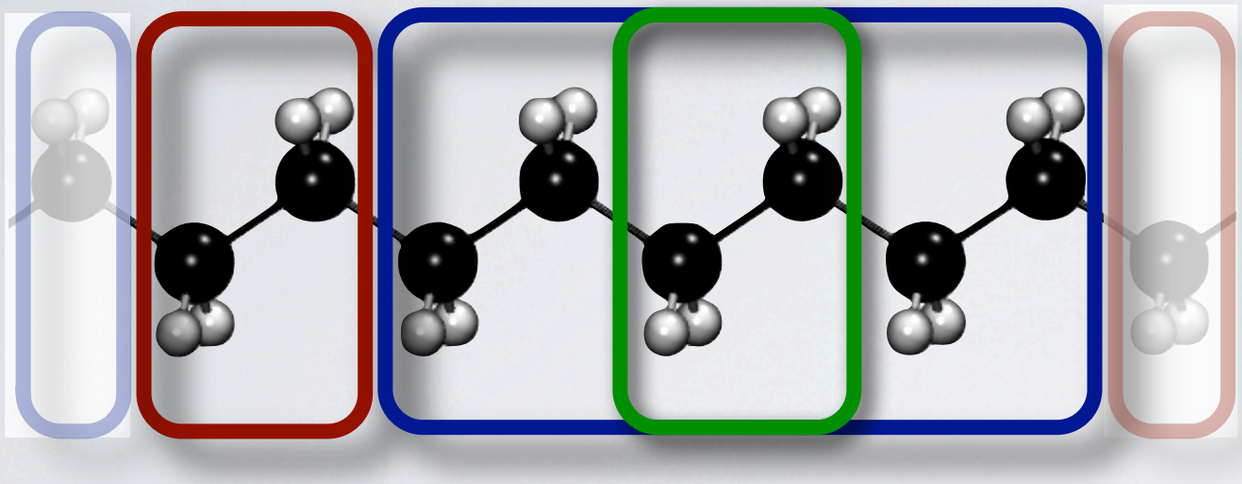
Start the calculation on **4 CPUs** and **redirect**
the **output** into **$HOME/MD.out**

```
mpirun -np 4 aims.hands-on-2011.scalapack.mpi.x > $HOME/MD.out
```

Please remember to start the run before leaving!

III. Evaluation of the Calculations

Monitor temperature of central $(CH_2)_2$



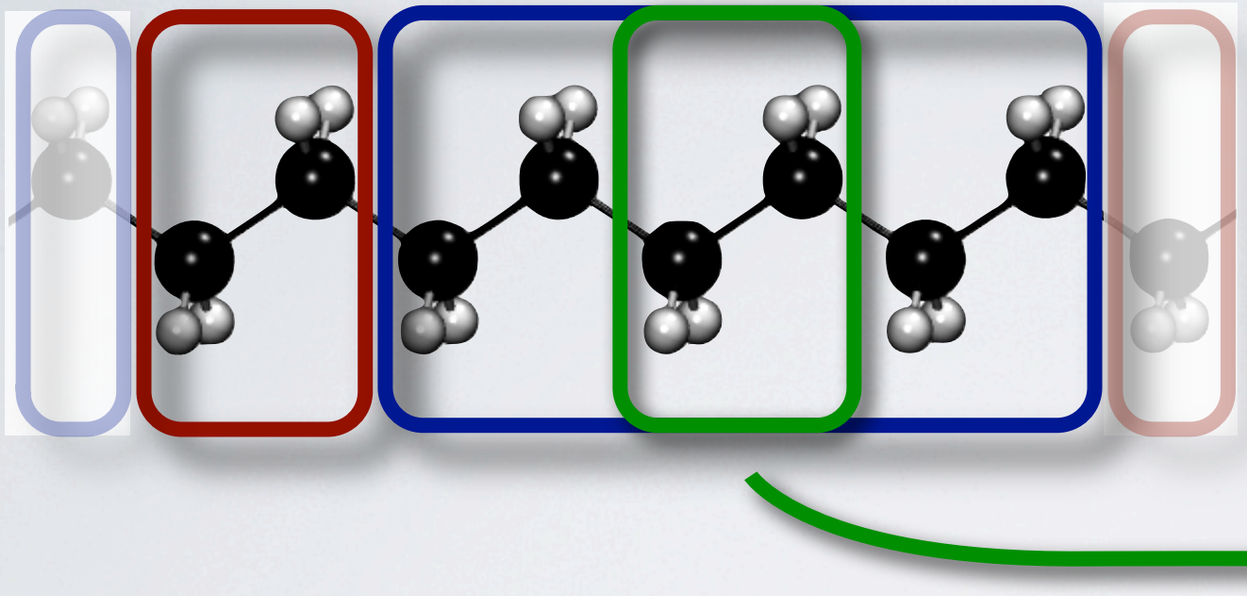
(A) Use the script

./extract_temperature_central_cell.pl MD.out

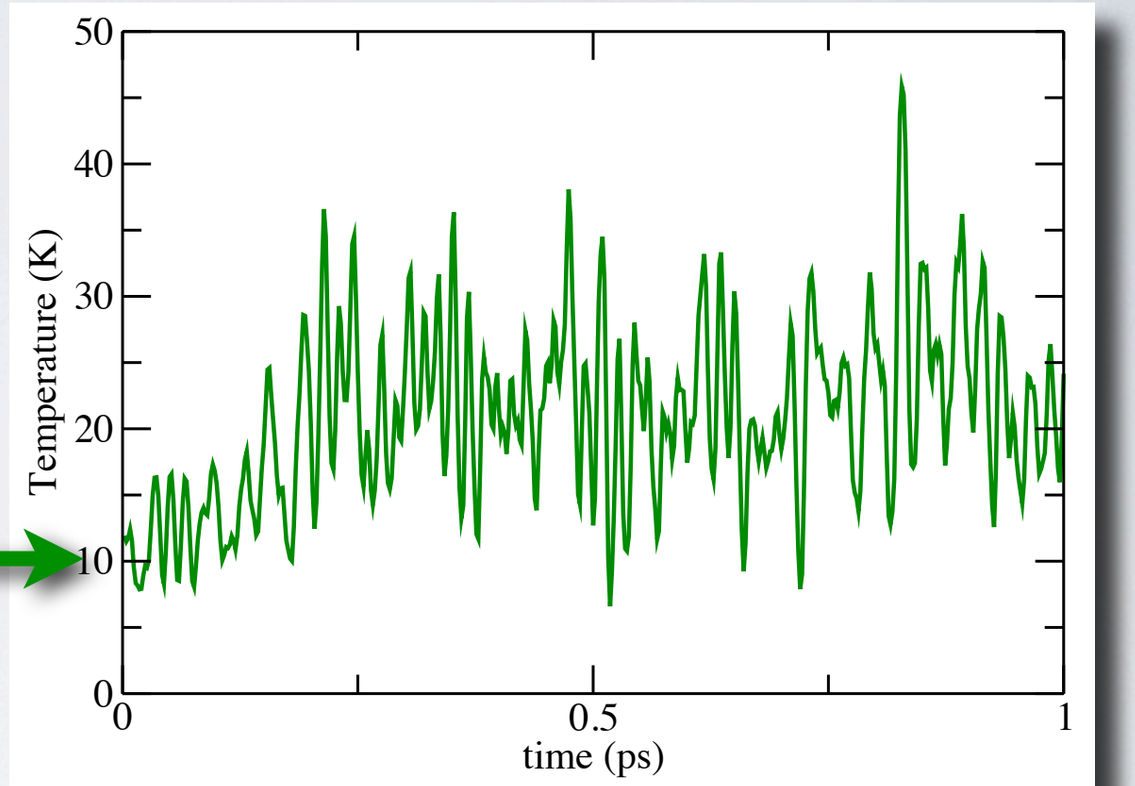
to extract the temperature of the central $(CH_2)_2$ group.

(B) Plot the output MD.out.temperature.dat with Xmgrace.

Monitor temperature of central $(CH_2)_2$



Monitor temperature of the central $(CH_2)_2$



The finite number of **atoms** leads to large temperature fluctuations.

Average over multiple runs

You can find ALL trajectories in
$HOME/results/tutorial5/exercise_6/

(A) Use the script

./summarize_and_average.sh

to average over **ALL** trajectories of **ALL** groups.

(B) Open the output with

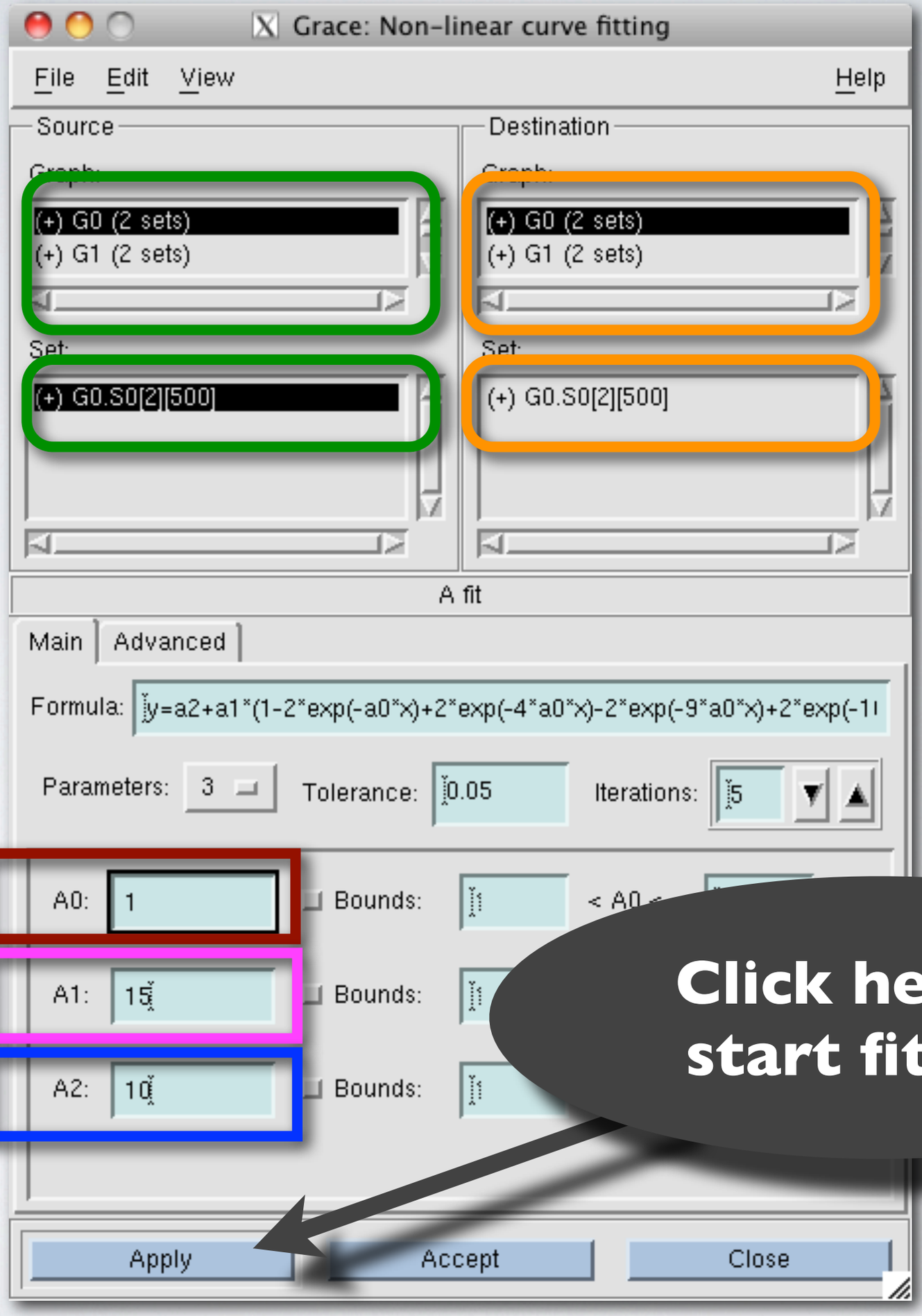
xmgrace -batch fitting.grace AverageTemperatures.agr

(C) Fit the individual graphs with Xmgrace‘s

Data -> Transformations -> Non-linear Curve Fitting

Graph and set that is fitted!

Graph and set to which the fit is written!



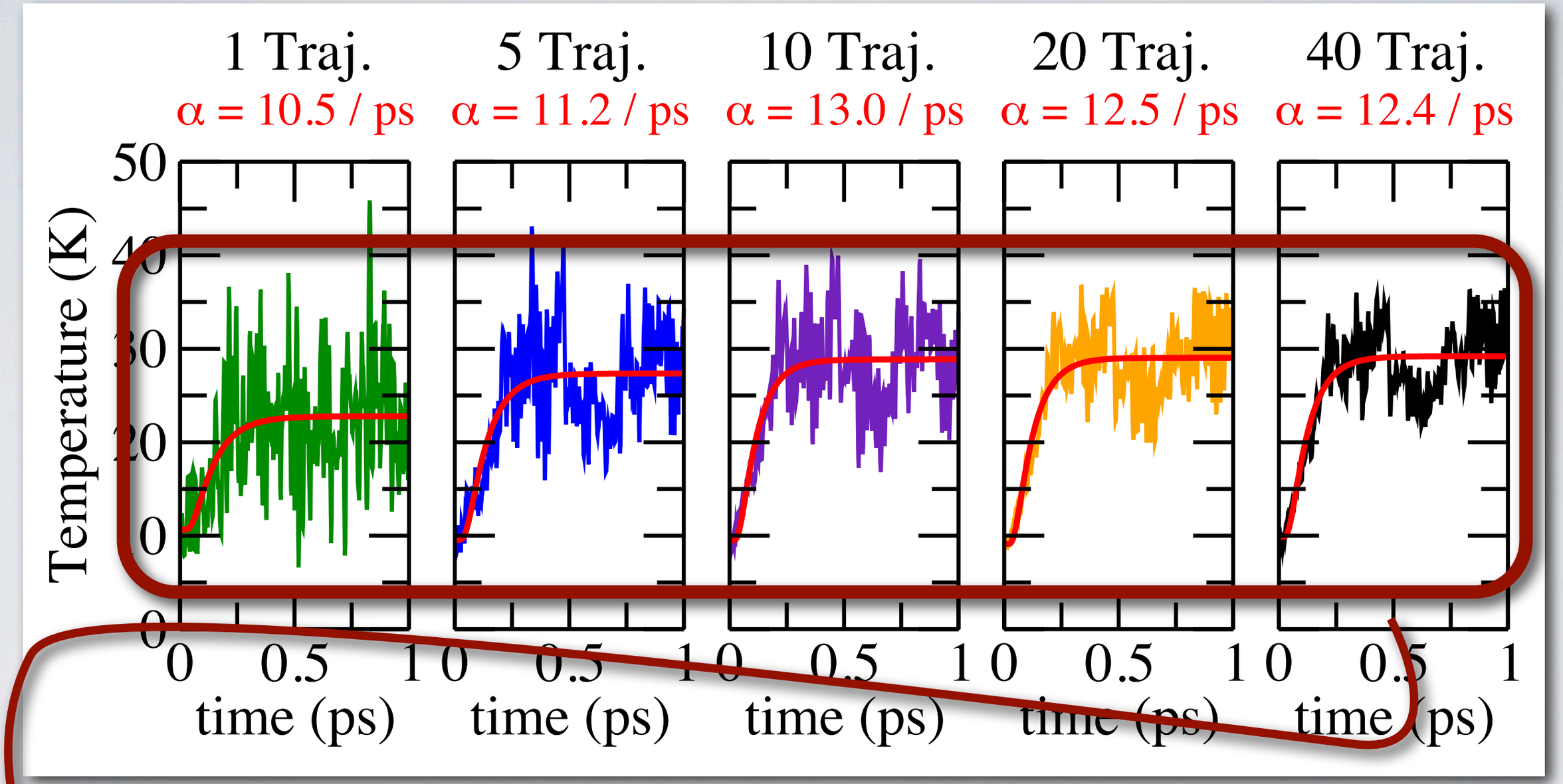
$\alpha\pi^2/x^2$

ΔT

T_{cold}

Click here to start fitting!

Laser-Flash-Simulations



Fit to

$$T(x,t) = T_{cold} + (T_{final} - T_{cold}) \sum_n (-1)^n \exp\left(-n^2 \pi^2 \alpha\, t\right)$$