タンパク質中の不均一な熱輸送物性の解析

Non-uniform thermal transport properties in proteins

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We have studied thermal transport properties in proteins using molecular simulations [1-7]. Within protein molecules, tightly packed amino acid residues interact with each other through heat and energy exchanges. We illustrate non-uniform heat flow in proteins with our own model based on "local heat/energy conductivity" between each residue pair.

Native contacts in proteins are classified into nonpolar, polar, and charged types. Harmonic spring picture applies to vibrational energy transfer (VET) through nonpolar and polar contacts, and VET rates vary inversely with the variance of the contact length: whereas diffusion picture is relevant to VET through charged contacts and VET rates correlate inversely with the mean-square-distance between charged atoms of a residue pair.

The *CURP* program [8] permits to compute inter-residue flow or energy/heat and atomic stress tensor in a protein, given atomic coordinates and velocity trajectories obtained through molecular dynamics (MD). Energy flow data permit to picture an inter-reidue Energy Exchange Network (EEN) as a graph. For interactive analysis of EEN graphs using pointing devices, a new visualization tool, *EEN VIEWER*, with JavaScript and Python codes (https://youtu.be/zCXmIXskBFE) is under development.

We implemented an accelerated CURP code with the OpenACC library for GPGPU (Fig. 1) As a result, the computation time of the heat current auto-correlation functions was accelerated by 98.4% for a test case (Fig. 2). This program was applied to a sensory domain of an oxygen sensor protein, FixL, which forms dimer in solution. We examined the non-uniform residue-residue interactions at the dimer interface by using EEN map (Fig. 3).

```
! << Calculate auto-correlation function >>
!$acc data copyin(xss(:,:)) copyout(acf(:,:))
!$acc kernels
do icom=1, ncom
   do iacf=1, nacf
      a=0.0d0
      do ifrm_beg=first, nfrm_beg, shift

         a = a + xss(ifrm_beg,icom) * xss(ifrm_beg+(iacf-1)*interval,icom)

      end do
      acf(iacf,icom) = a
   end do
end do ! samples of one file data
!$acc end kernels
!$acc end data

nsam = (nfrm_beg-first)/shift + 1
! print*, first, nfrm_beg, nsam
acf(:,:) = acf(:,:) / real(nsam)
```

Figure 1.

CURP code with OpenACC directives

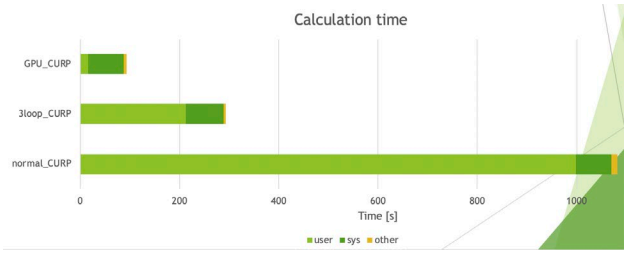

Figure 2. Acceleration by GPGPU computing

The total processing time for the evaluation of the time correlation function of heat current vectors was reduced by 98.4 % (top) compared to the original curp code (bottom).

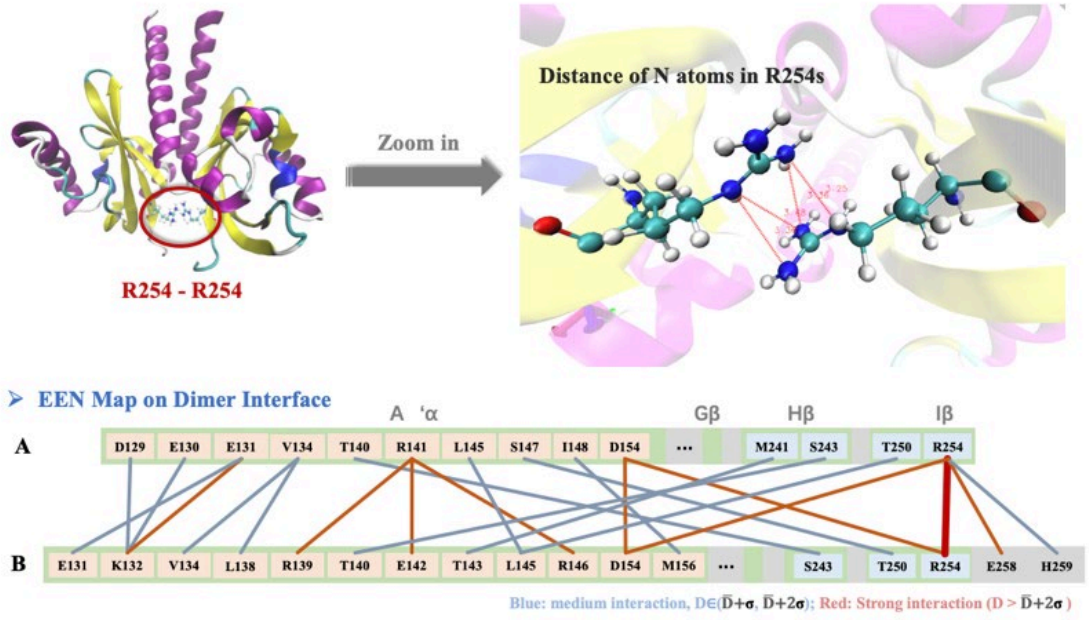

Figure 3. Interaction at the dimer interface of FixL

We performed conformational sampling of the FixL dimer (top left) using equilibrium molecular dynamics simulations with the Amber program, and conducted multiple NVE simulations starting 200 different initial conditions. We obtained time series of energy/heat current between residue pairs in contact using these NVE trajectories, and calculated their transport coefficients, *D*, based on the Green-Kubo formalism using the CURP program. As a result, we identified strong (red) and medium (blue) interactions (bottom panel). Interestingly, a pair of positively charged residues (R254) was hold together (top right) with each residue being attracted by the negatively charged D154 on the other side.

References

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