Science & Technology Facilities Council
Daresbury Laboratory

DL_POLY_4: A bird's eye view

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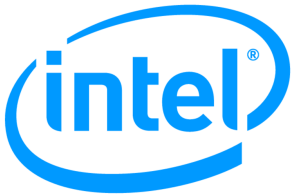
Hartree Centre

Science & Technology Facilities Council

NCSA

NATIONAL CENTRE FOR SUPERCOMPUTING APPLICATIONS



BAYNCORE

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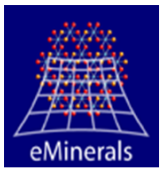
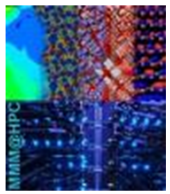
Ilian Todorov, Bill Smith
Ian Bush, R Davidchak, Michael Seaton, Andrey Brukhno





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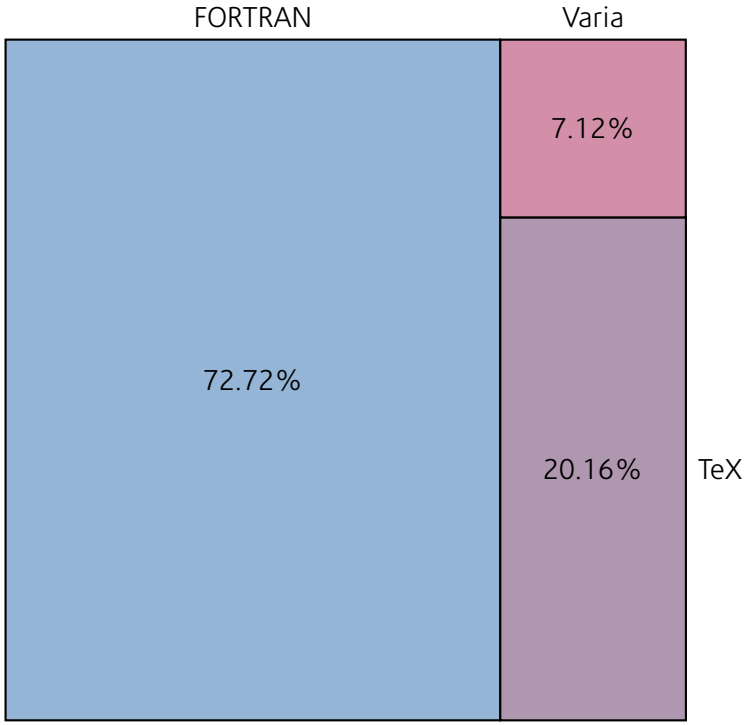
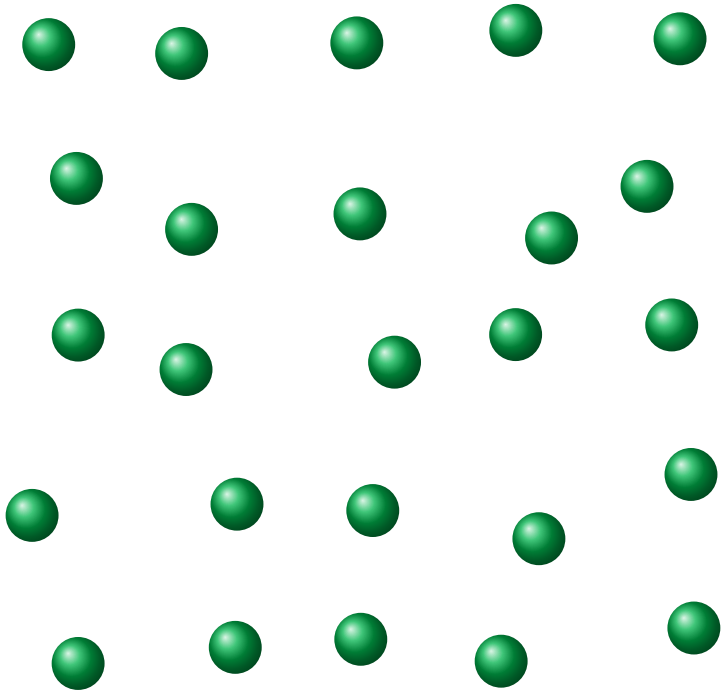


- classical molecular dynamics code developped at Daresbury Lab mainly by I T Todorov and W Smith
- an entire zoology of time integrators and ensembles
- Modern Fortran with MPI and OpenMP.
- suitable for simulations from biological systems to materials under extreme conditions
- coding style: very physicists oriented…

The Model



$$\mathbf{r} = \{\mathbf{r}_i\}_{i=1,N}, \quad \mathbf{v} = \{\mathbf{v}_i\}_{i=1,N}$$

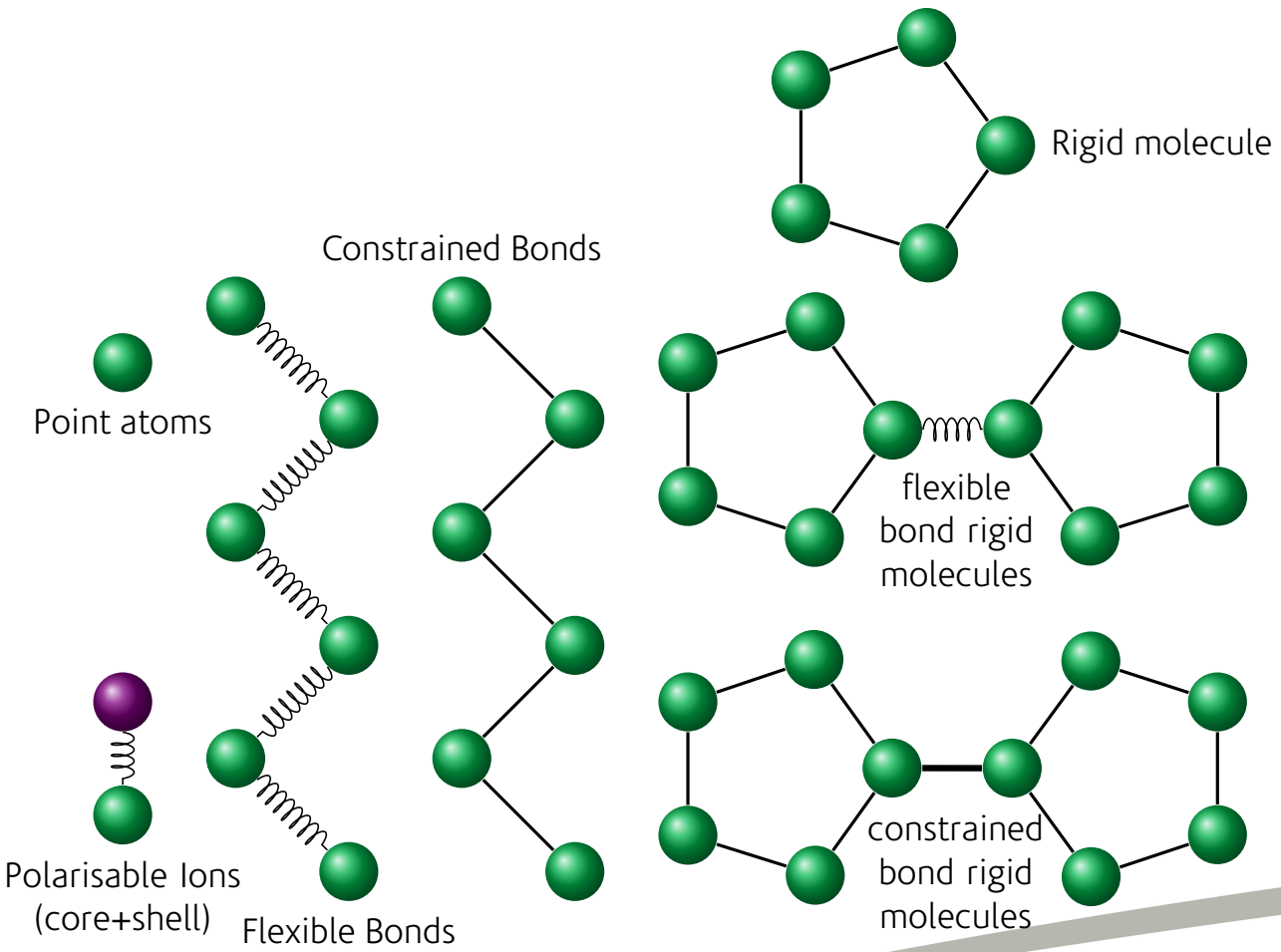
$$\mathscr{L}(\mathbf{r}(t), \mathbf{v}(t)) = \sum_{i=1}^{N} \frac{m_i \mathbf{v}_i \cdot \mathbf{v}_i}{2} - V(\mathbf{r})$$

$$\frac{d}{dt}\left(\frac{\partial \mathscr{L}}{\partial v_i^\alpha}\right) = \frac{\partial \mathscr{L}}{\partial r_i^\alpha}$$

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i$$

$$\mathbf{F}_i = -\nabla_i V(\mathbf{r}_1, \ldots, \mathbf{r}_N)$$

The Model


Rigid molecule
Constrained Bonds
Point atoms
flexible
bond rigid
molecules
Polarisable Ions
(core+shell)
Flexible Bonds
constrained
bond rigid
molecules

The Model

$$
\begin{aligned}
V(\mathbf{r}_1,\ldots,\mathbf{r}_N) = & \sum_{i,j=1}^{N}{}' V_{pair}\left(|\mathbf{r}_i-\mathbf{r}_j|\right) + \sum_{i,j=1}^{N}{}' \frac{q_i q_j}{4\pi\varepsilon_0\varepsilon_r|\mathbf{r}_i-\mathbf{r}_j|} + \\
& + \sum_{i,j,k=1}^{N}{}' V_{3b}\left(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k\right) + \sum_{i,j,k,l=1}^{N}{}' V_{4b}\left(\mathbf{r}_i,\mathbf{r}_j,\mathbf{r}_k,\mathbf{r}_l\right) \\
& + \varepsilon_{metal}\left(\sum_{i,j=1}^{N}{}' V_m\left(|\mathbf{r}_i-\mathbf{r}_j|\right) + \sum_{i=1}^{N} F\left(\sum_{i,j=1}^{N}{}' \rho_{ij}\left(|\mathbf{r}_i-\mathbf{r}_j|\right)\right)\right) + \\
& + \sum_{i_{ab}=1}^{N_{bonds}} V_{bond}(i_{ab},\mathbf{r}_a,\mathbf{r}_b) + \sum_{i_{abc}=1}^{N_{angles}} V_{angle}(i_{abc},\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_c) + \\
& + \sum_{i_{abcd}=1}^{N_{dihedrals}} V_{dihedral}(i_{abcd},\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_c,\mathbf{r}_d) + \sum_{i_{abcd}=1}^{N_{inverse}} V_{inverse}(i_{abcd},\mathbf{r}_a,\mathbf{r}_b,\mathbf{r}_c,\mathbf{r}_d) + \\
& + \sum_{i_a}^{N_{tethers}} V_{tether}(i_a,\mathbf{r}_a{}^{\tau=t},\mathbf{r}_a{}^{\tau=0}) + \sum_{i_{cs}=1}^{N_{shells}} V_{core-shell}(i_{cs},\mathbf{r}_c,\mathbf{r}_s) + \sum_{i=1}^{N}\varphi_{ext}(\mathbf{r}_i)
\end{aligned}
$$

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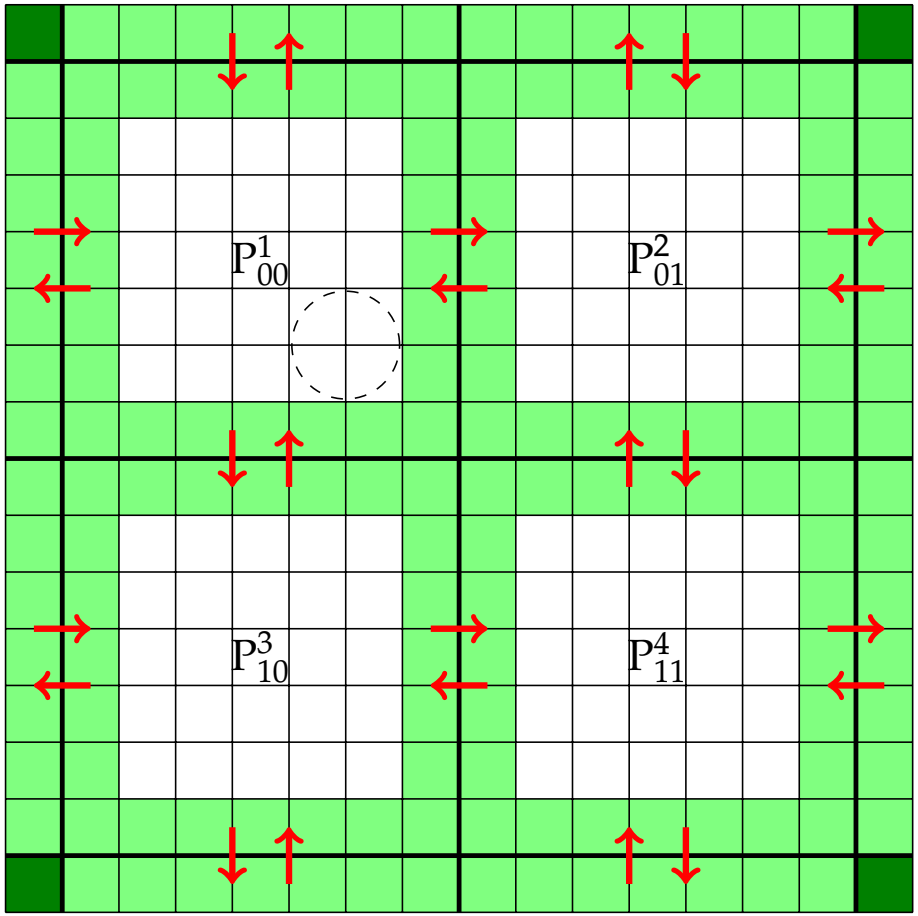
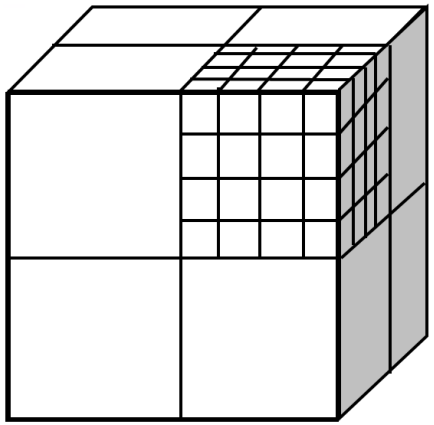
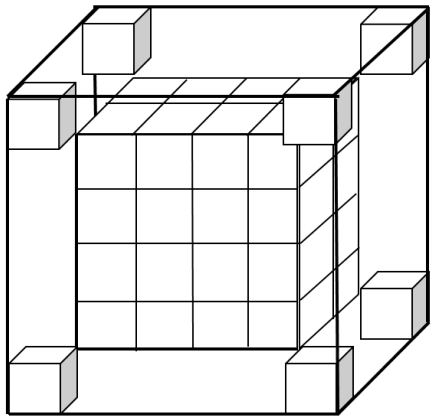
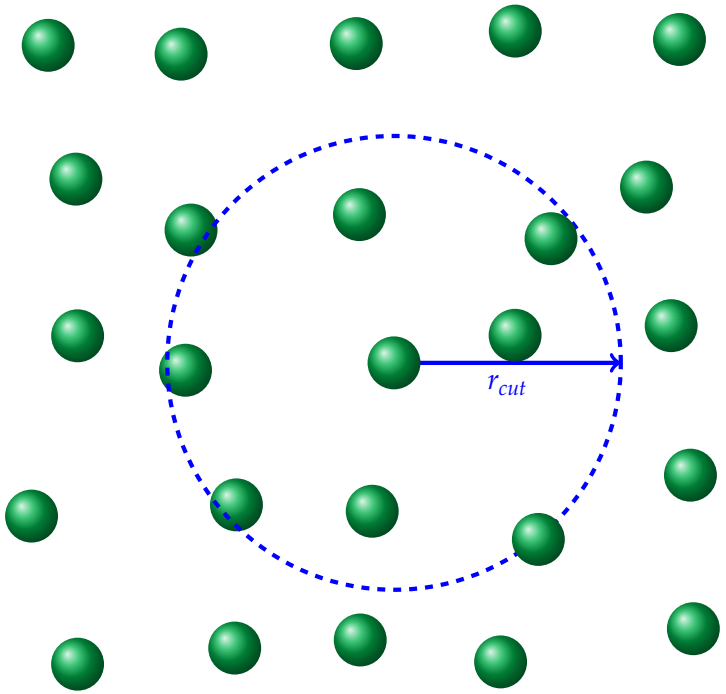
Domain Decomposition

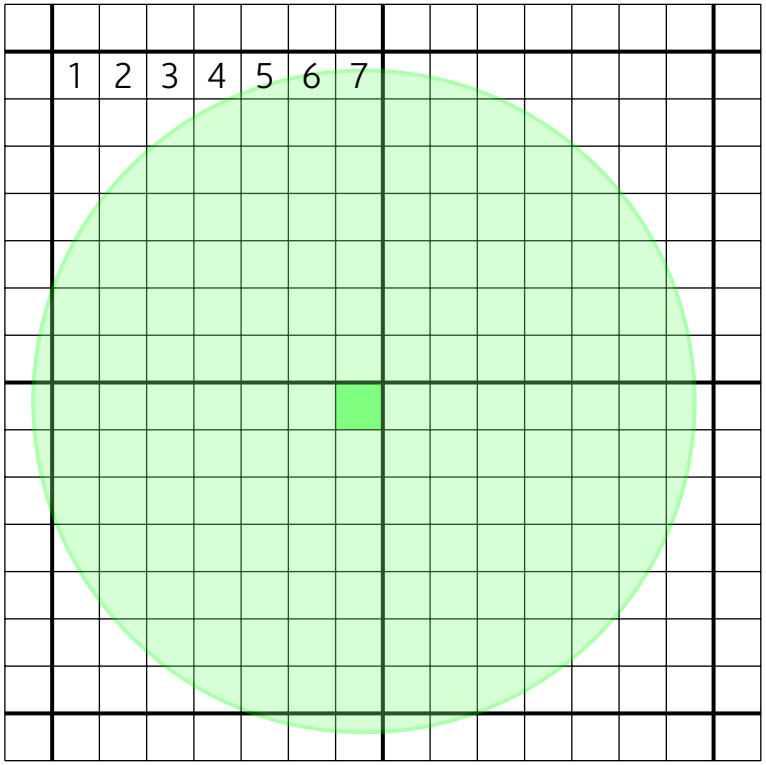






Linked cells





Basic Integrator

read **r**
read/generate **v**
calculate forces $\mathbf{F}(t=0)$
do it=1,timesteps

$$\mathbf{v}\left(t+\frac{\Delta t}{2}\right)=\mathbf{v}(t)+\frac{\Delta t}{2}\frac{\mathbf{F}(t)}{m}$$

$$\mathbf{r}(t+\Delta t)=\mathbf{r}(t)+\frac{\Delta t}{2}\mathbf{v}\left(t+\frac{\Delta t}{2}\right)$$

correct $\mathbf{r}(t+\Delta t)$
calculate $\mathbf{F}(t+\Delta t)$

$$\mathbf{v}(t+\Delta t)=\mathbf{v}\left(t+\frac{\Delta t}{2}\right)+\frac{\Delta t}{2}\frac{\mathbf{F}(t+\Delta t)}{m}$$

correct $\mathbf{v}(t+\Delta t)$
calculate statistics
end
final statistics

generate linked cell lists
calculate long range contributions
do i=1,nAtoms
  do j in Neighbours of i
    calculate force on i due to j
  end
end

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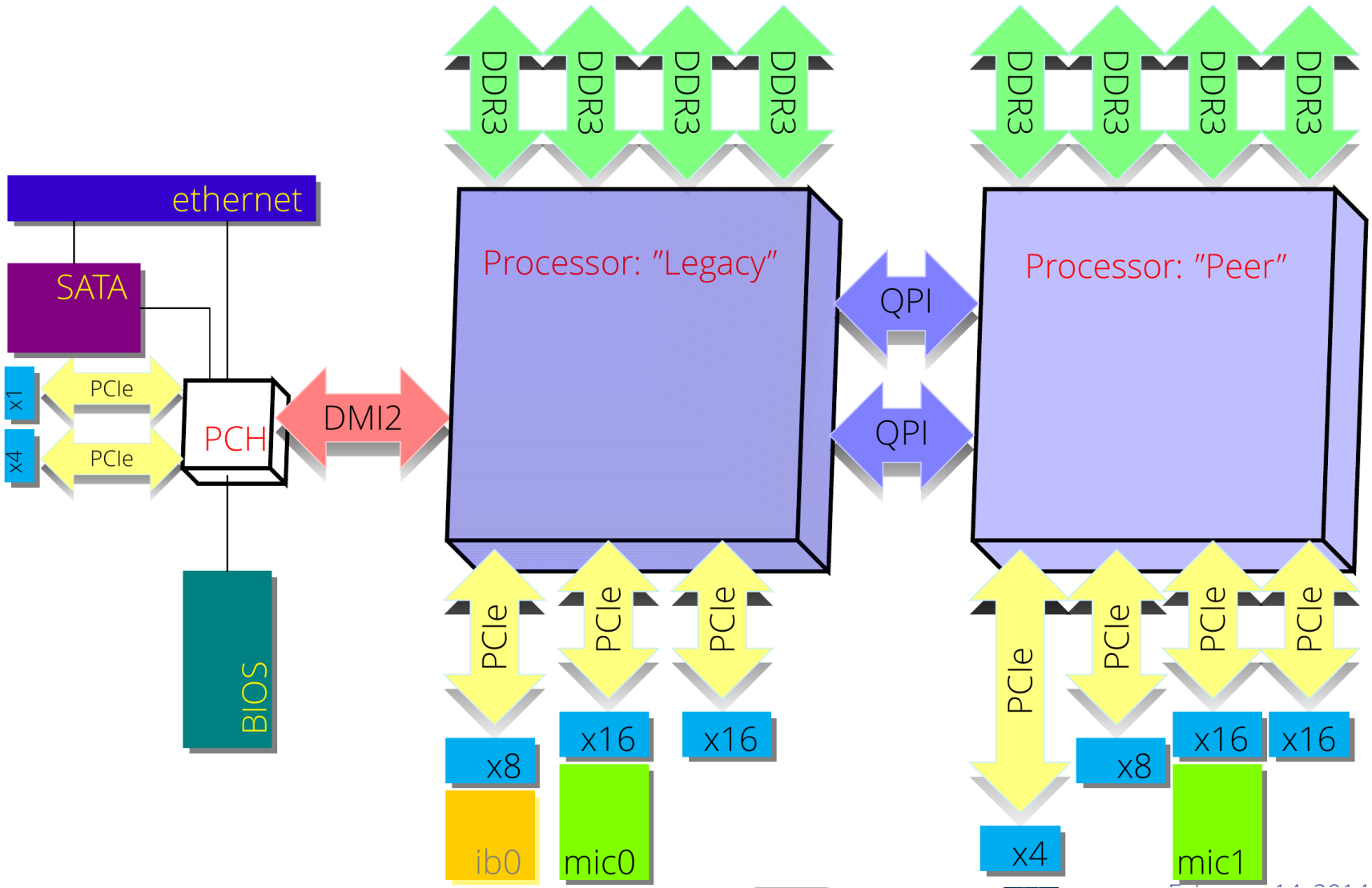
Knights Corner in a node



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Q&A

Exercises

ssh -p 1022 <yourusername>@gw.avitohol.acad.bg

ls /home/alin/sofia/

DLPOLYIntro.pdf
dl-poly-stfc-omp.tar.xz
dl-poly-stfc-phi.tar.xz
Exercises.pdf
gramidicin
SC15-MolSimSoftware_paper_3-AlinMarinv2.pdf
scripts

$$x_{n+1} = 108 - \frac{815 - \frac{1500}{x_{n-1}}}{x_n} \quad with \quad x_0 = 4,\ x_1 = \frac{17}{4}$$

$$x_{42} = ?$$