

oneAPI Technical Advisory Board Meeting

December 16, 2020 Virtual Meeting

Agenda

Duration	Topics
10 minutes	oneAPI: how we got here, where we are going
40 minutes	Break out sessions
5 minutes	Closing

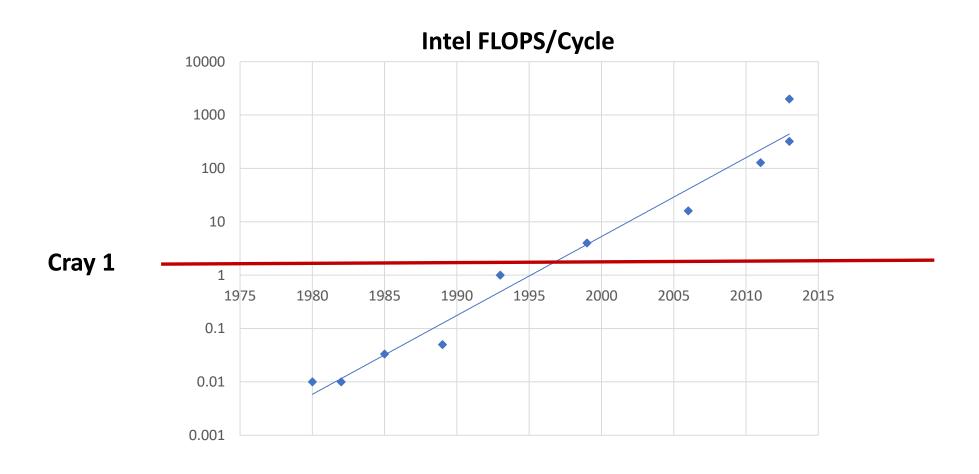
Welcome and Thanks

• A unique opportunity to steer the parallel programming ecosystem

- A problem worth solving
 - Multi-architecture, avoiding lock-in to 1 specific hardware architecture
 - Direct and library-based programming
 - Extending existing models
 - Performant

Your leadership, input, and feedback is critical

Moore's Law and compilers



2007: LIBOR loop nest

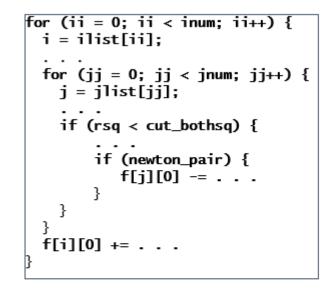
```
for (path=0; path<npath; path++) {</pre>
for(n=0; n<Nmat; n++) {
  for (i=n+1; i<N; i++) {
    lam = lambda[i-n-1];
    con1 = delta*lam;
  v += (con1*L[i])/(1.0+delta*L[i]);
    vrat = exp(con(*v) lam*(sqez-0.5*con1));
    L[i] = L[i]*vrat;
```

Outer loop parallel

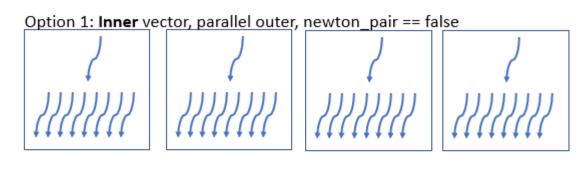
Inner loop sequential

2017: SIMT vs Threads & vectors

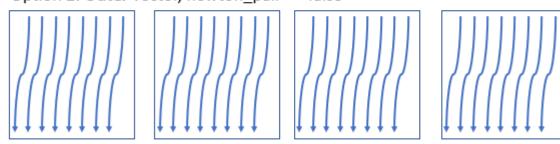
CHARMM (Bio) Force-Field from Baseline LAMMPS



	GPU	CPU
1. Inner	92.71%	84.61%
2. Outer	100.00%	84.61%
3. Privatize	66.97%	100.00%
4. Atomic	91.21%	59.14%



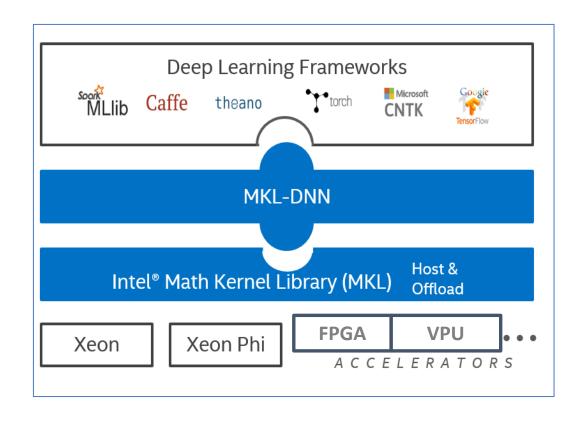
Option 2: Outer vector, newton pair == false

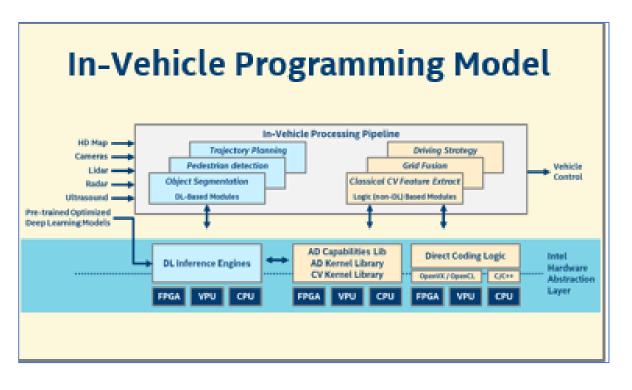


Option 3: **Privatize,** inner vector, parallel outer, newton_pair == true

Option 4: **Atomic**, inner vector, parallel outer, newton_pair == true

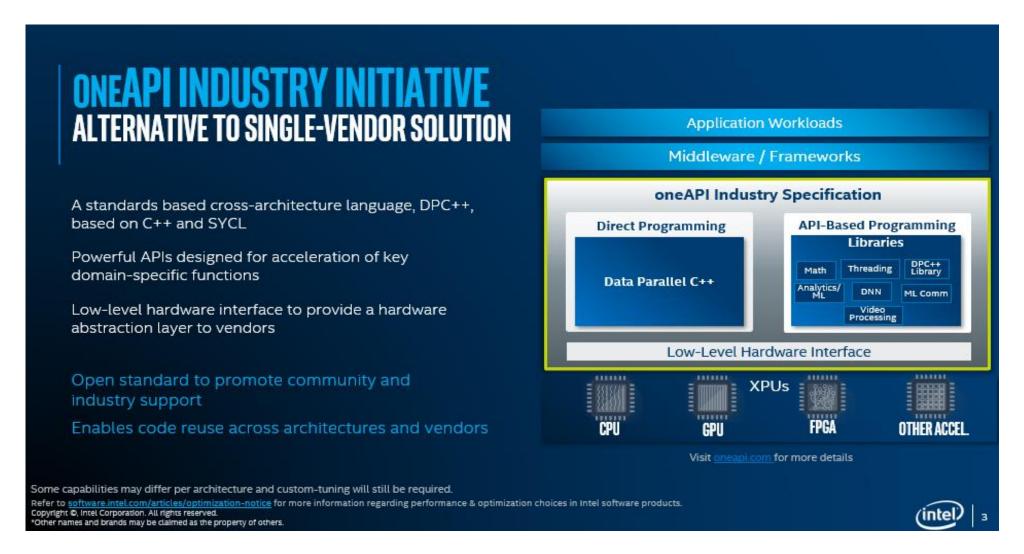
2017: API programming and direct programming



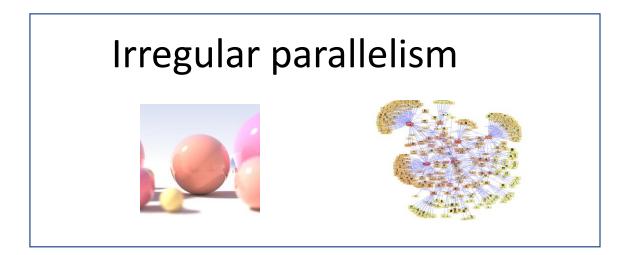


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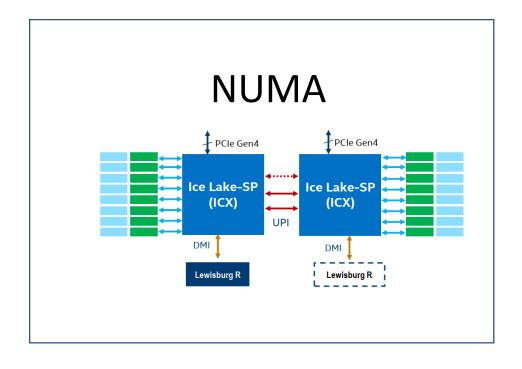
2019: oneAPI



2021: Issues to address







Give the break out information