My experience with OpenMP off-loading C++ classes

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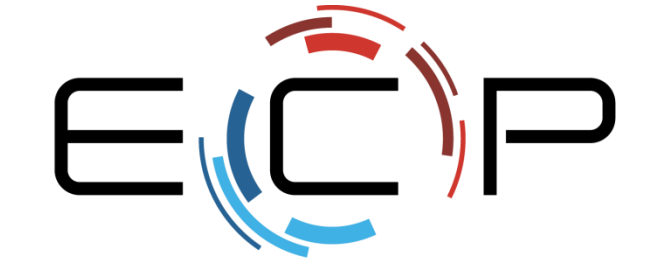

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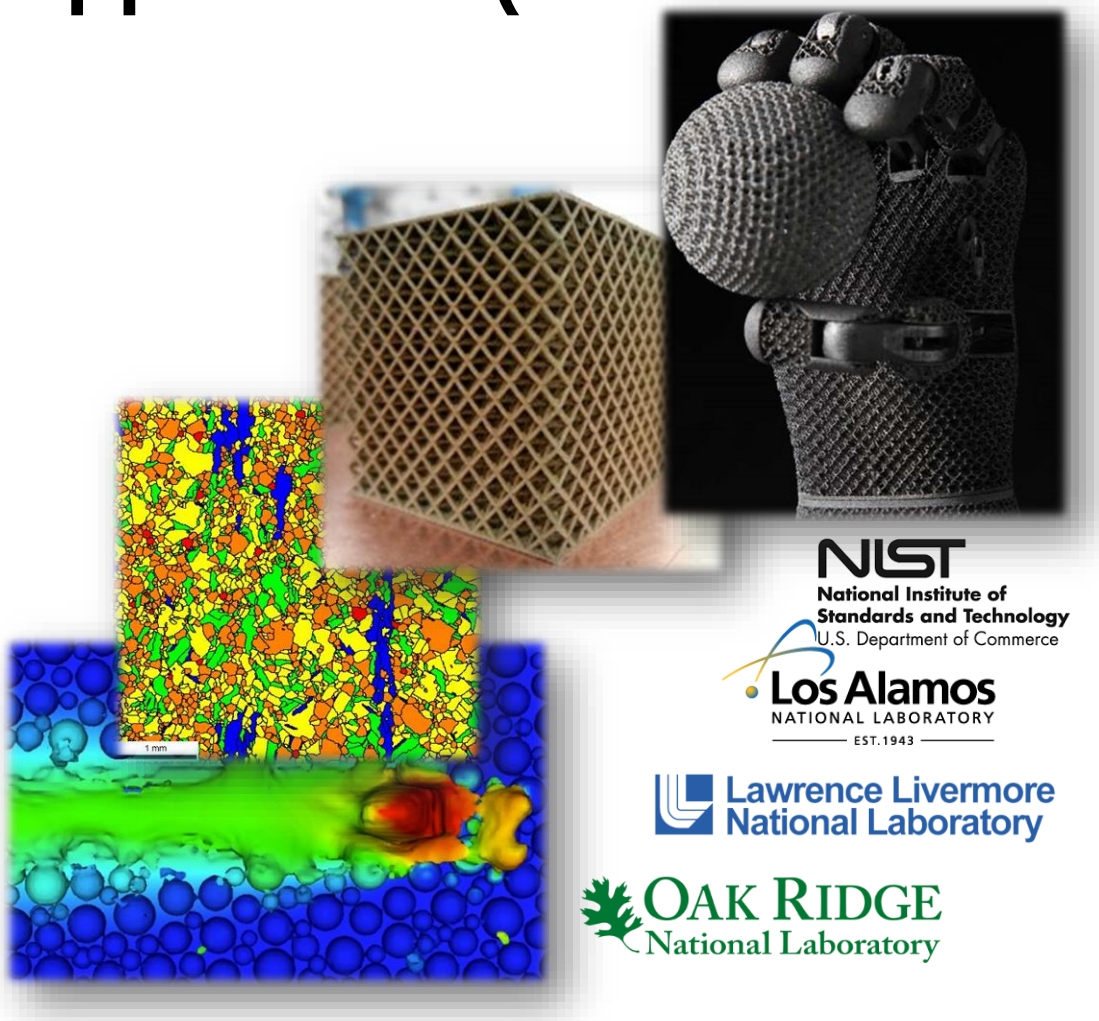
Context: ExaAM project, an ECP application (PI: John Turner, ORNL)

- What is Additive manufacturing?
  - The process of joining materials to make objects from 3D model data, usually layer upon layer, as opposed to subtractive manufacturing methodologies
- Goal
  - Improve quality, reliability, and application breadth of additive manufacturing for metallic alloys
- Computational approach
  - Coupling multiple codes modeling various length-scales



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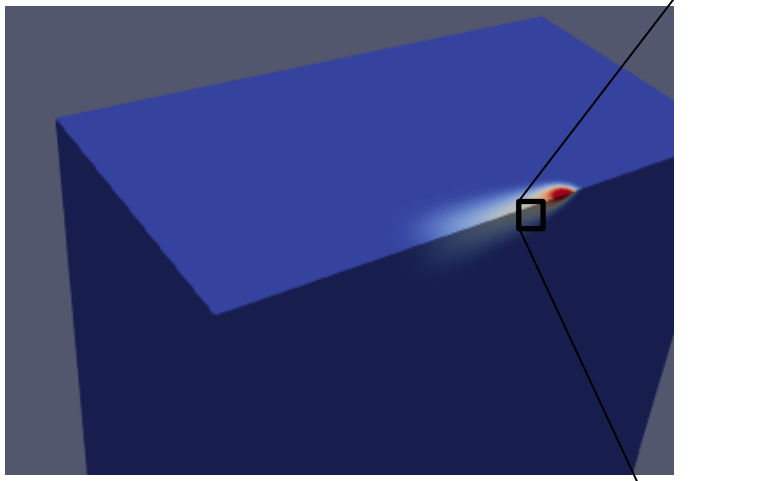
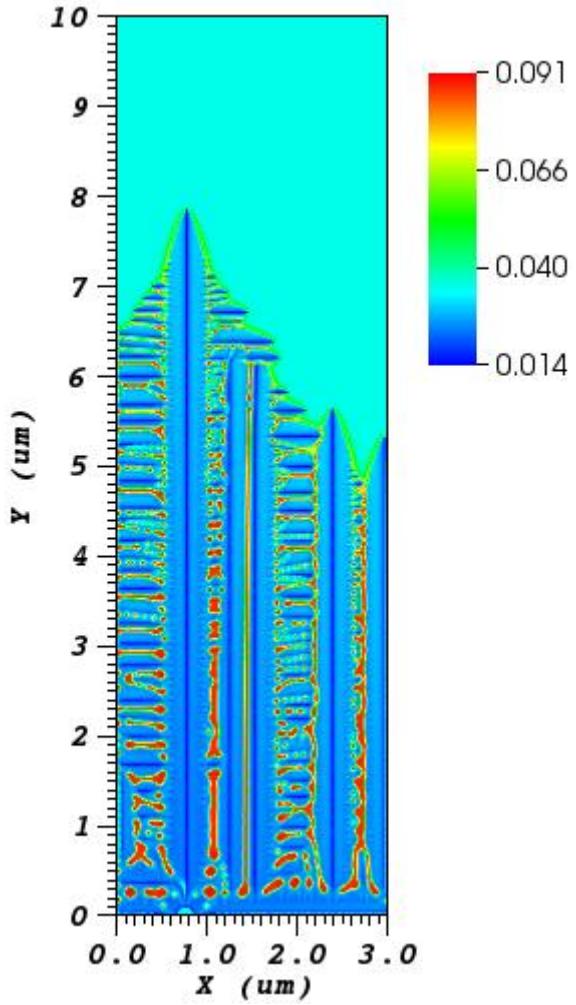
ECP EXASCALE COMPUTING PROJECT

Fine-scale Microstructure using Phase-field model



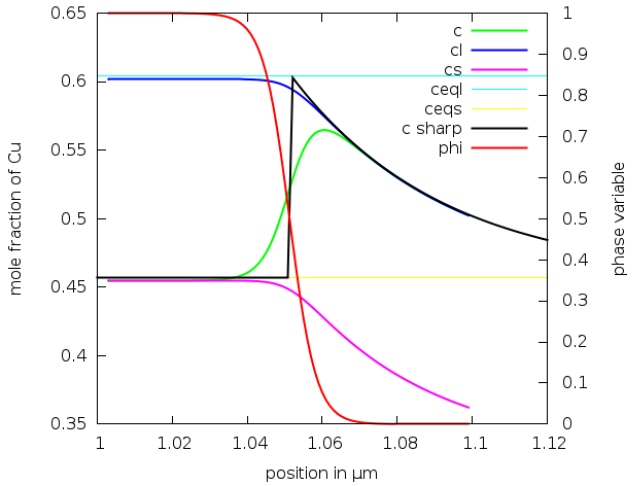


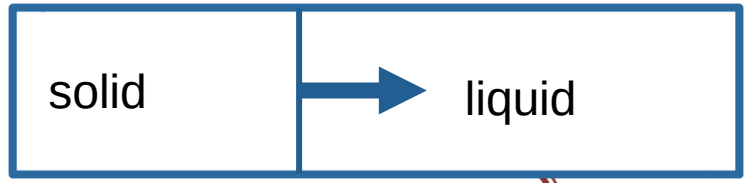
Phase-field equation

$$\frac{\partial \phi}{\partial t} = M\left[\varepsilon^2 \nabla^2 \phi + W\phi(1-\phi)(1-2\phi) + \frac{\partial f}{\partial \phi}\right]$$

+ a few other coupled equations

C++11 Code: AMPE
https://github.com/LLNL/AMPE





KKS phase-field model for alloys [Kim, Kim, Suzuki, Phys Rev E (1999)]

- Case of binary alloy
  - At every mesh point of discretization grid, given ϕ (phase fraction) and c (alloy composition), solve a set of nonlinear equations for c_s and c_L using a Newton solver

$$c = \phi c_S + [1 - \phi] c_L$$

$$\frac{\partial f^s}{\partial c_S} = \frac{\partial f^L}{\partial c_L}$$

- Ternary alloy
  - Similar with 4 unknowns and 4 equations
- f^S and f^L known functions, parameterized with 10+ parameters each

Solvers initial C++ implementation

- Base class
  - Newton solver
  - Pure virtual functions to compute right handside and Jacobian
- Derived class
  - Implements specific right handside and Jacobian computation
- CPU code

$$\phi c_S + [1-\phi] c_L - c = 0$$

$$\frac{\partial f^S}{\partial c_S} - \frac{\partial f^L}{\partial c_L} = 0$$

```
#pragma omp parallel for
for(int i=0;i<N;i++)
{
        BinaryAlloySolver s(T[i]);
        double x[2];
        s.solve(phi[i],c[i], x);
        …
}
```

What can I do or not do with OpenMP4.5 offload?

- Things I knew I could not use within OpenMP region
  - STL
- Things I suspected I could not use within OpenMP region
  - virtual functions
  - assert()
- Things I discovered I could not use within OpenMP region
  - Classes with non-trivial constructors/destructors, or even classes with declared a constructor and/or destructor

Strategy to offload code

- Platform: Summit @OLCF
- Compiler: gcc/10.2.0
- Compiler error messages not very specific/informative …
  - No info on which specific function or what cannot be offloaded
- Use “toy” code to test what the compiler let me do or not
  - “OpenMP Application Programming Interface, Examples”, Version 4.5.0 – November 2016
  - Step-by-step move closer to target code design

Moving towards a working C++ code

- Remove STL, assert
- Make constructors/destructors trivial
  - Add setup functions to initialize objects
- Use Curiously Recurring Template Pattern (CRTP) to avoid virtual functions

Limited C++: C code + class encapsulation + templates

Working Code

```
template <unsigned int Dimension, class SolverType>
Class NewtonSolver
{
#pragma omp declare target
    void internalRHS(const double* const x, double* const fvec)
    {
        static_cast<SolverType*>(this)->RHS(x, fvec);
    }
…
#pragma omp end declare target
}
```

```
class CALPHADConcSolverBinary : public NewtonSolver<2, CALPHADConcSolverBinary>
{
public:
#pragma omp declare target
    int ComputeConcentration(double* const conc, const double tol,
        const int max_iters, const double alpha = 1.)
    {
        return NewtonSolver::ComputeSolution(conc, tol, max_iters, alpha);
    }
#pragma omp end declare target


…
}
```

Driver code

```
# pragma omp target \
    map (to: sol ) map ( tofrom: xdev ) \
    map (to: fA, fB, Lmix_L, Lmix_A) \
    map (to: RTinv), map ( from: nits)
{
#pragma omp teams distribute parallel for
for(int i=0;i<N;i++)
{
    xdev[2*i]=sol[0];
    xdev[2*i+1]=sol[1];

    double hphi = 0.5+i*deviation;
    double c0 = 0.3;

    class Thermo4PFM::CALPHADConcSolverBinary solver;
    solver.setup(c0, hphi, RTinv, Lmix_L, Lmix_A, fA, fB);
    nits[i] = solver.ComputeConcentration(&xdev[2*i], 1.e-8, 50);
}
}
```

Performance

- 4.5X speedup GPU over CPU on Summit for ternary alloy problem (4 coupled equations)
  - 6 GPU offload vs. 42 OpenMP CPU threads
- Performance currently limited by GPU registers memory
  - Planning to replace some “double” with “float” to reduce memory requirements

Conclusion

- Working solution for gcc on Summit
  - Requires some non-trivial code changes
  - Still debugging some classes…
- Open source soon
  - https://github.com/ORNL/Thermo4PFM
- Decent performance, to be improved with mixed precision
- XL compiler not working for me at the moment
- Better (and user friendly) documentation about porting C++ classes would be really helpful
  - Probably dependent on compiler, compiler version,…
- More targeted error messages at compile time would help too…

Acknowledgements

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