Title

Carbon3D HPC4Mfg Final Report

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Carbon3D HPC4Mfg Final Report

Project Title: Development of a Multi-physics Model to Optimize Continuous Liquid Interface Production (CLIP) for Additive Manufacturing

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Computational Resources used for Project:

System	Time (MCH)	Commercial Software	Custom Software
NERSC Edison	85,000		Chombo-based modeling code
Local workstations			same

Executive Summary (1 page or less):
Non-proprietary, publishable *summary of problem being addressed, why problem is important to the energy future of the US, plan to address problem, and the impact the solution will have on the national energy. Results, Implementation, Future work.*

Continuous Liquid Interface Production (CLIP) is poised to bring additive manufacturing to multiple American manufacturing sectors owing to its unique combination of rapid print speeds and material options that resemble injection molding thermoplastics. In spite of these benefits, CLIP is still a maturing process. To improve our understanding and control of the process, this project developed a multi-physics computational model that encompasses the coupled chemical-physical processes of photopolymerization and fluid flow to predict part outcomes. A physically predictive model can enable rapid optimization of CLIP and reduce the current cycle time and waste associated with optimization by four-fold. Ultimately, this effort will help open the U.S. $400B plastic manufacturing industry to the key benefits of additive manufacturing, namely mass customization, unlimited design space, and a cost- and energy-effective path to mainstream manufacturing.

In the course of the project we produced a model which coupled fluid-flow, species transport, and photochemistry to model the Carbon CLIP process. As the development proceeded, we validated the code against theory and experiments. The resulting code was transferred to Carbon, and we expect it to be a useful part of their modeling capability. Future work includes improvements to the fluid solver's robustness and performance, along with the addition of additional physics models.

Introduction:

Motivation:
Carbon, Inc. (http://carbon3d.com) is an additive manufacturing company with a new method using unique polymeric materials in a Continuous Liquid Interface Production (CLIP) process (illustrated in Figure 1). Our focus is on modeling the dynamic reacting flow problem in the vicinity of the UV window where the part polymerization depends upon the local flow, species, and temperature fields. To that end, we have developed a multi-physics, physically-predictive model that encompasses the coupled chemical-physical processes of photopolymerization, heat transport, and fluid flow. The adaptive mesh refinement (AMR) capabilities developed at LBNL will enable efficient modeling of the wide range of spatial scales in play in the CLIP process. The HPC simulation capability created by LBNL for Carbon will help to diagnose CLIP process issues and optimize printing time and quality.

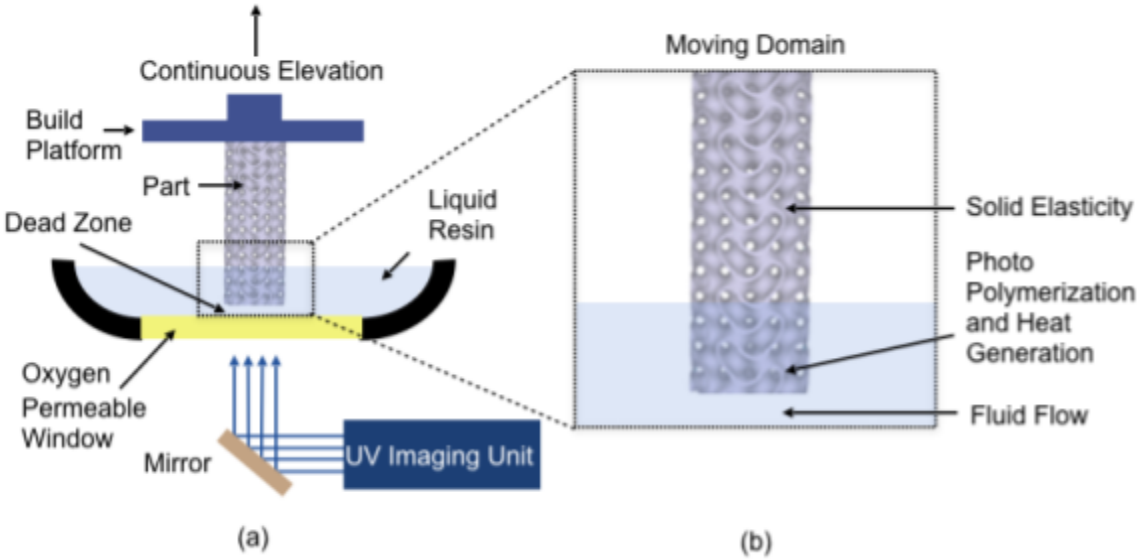


Figure 1: *Schematic of CLIP process: (a) UV light passing through an oxygen-permeable window causes polymerization of liquid resin bath, forming the part, which is continuously withdrawn. Oxygen passing through the window inhibits the reaction, producing a dead zone near the window and preventing the part from adhering to the window. (b) Inset illustrating which physical processes are relevant in the part, at the polymerization interface, and in the liquid resin. This HPC4Mfg project focused on the dynamics in the fluid and at the polymerization interface.*

Problem description:

For this award, we focused on modeling the dynamic reacting flow problem in the vicinity of the window-part interface to yield the local flow, species, and temperature fields for prescribed boundary conditions. The flow, heat transfer, and polymerization are coupled in several sub-steps that were individually validated and ultimately integrated to simulate the print of test geometries. These activities capture the core of the CLIP process and set the foundation for building a reduced-order model where every part being printed in the field could be quickly optimized. The key coupled physical processes include (Fig. 1b):

1. Viscous fluid flow into build zone.
2. Heat generation from photo-polymerization and heat dissipation.
3. Resin optical absorption and photo-polymerization

Carbon provided the full set of differential equations and constitutive relations that govern the process along with the data and measurement support for many of these input parameters. These were then given to LBNL to setup and solve through modifications of existing software, using the LBNL Chombo framework (http://Chombo.lbl.gov).

Approach:

The initial phase of the project consisted of a model and software design development phase, in which we produced algorithm and software design documents in collaboration with Carbon which outlined our planned approach, milestones, and relevant tests.

The software produced in this project built on existing code capabilities and ongoing research efforts in adaptive mesh refinement (AMR) approaches to modeling fluid dynamics, while developing a numerical model of Carbon's proprietary photopolymerization process in collaboration with Carbon. We then were able to couple the two capabilities together to create a coupled chemistry-fluid solver to model the Carbon process. There were three pieces of this model: the fluid solver, the species transport model, and the photochemistry module.

The *fluid solver* must be able to model a fluid with an embedded moving solid body with a mass flux of polymer through the polymerization boundary (the boundary between the part and the fluid). To do this, our initial plan was to use a higher-order Stokes-flow solver which used cut-cell Embedded-boundary (EB) discretizations to represent the complex geometries found in the part. However, that developmental solver wasn't robust enough to further develop within the time frame of this project, so a scheme based on Brinkman Penalization was used to enforce the moving-body boundary conditions in the fluid, along with a projection scheme to enforce the incompressibility constraint.

The s*pecies transport model* is a 4th-order advection-diffusion-reaction model for species transport (4 species: O2, monomer, radical, and photoinitiator) which employs operator splitting to compute hyperbolic advection terms explicitly, diffusion terms implicitly for numerical stability, while an ODE integrator updates the stiff photochemistry reaction terms. (Zhang, et al, 2012)

The *photochemistry module* implements the photo-reaction chemistry model provided by Carbon to model their proprietary reaction chemistry in the presence of a light source, and uses a ODE integrator for stiff problems from the Boost library.

Results:

In the development process, we implemented three tests of increasing complexity provided by Carbon:

1. Standalone Chemistry test: We first tested our chemistry implementation against Carbon-provided observations. We demonstrated good agreement, as shown in Figure 2.

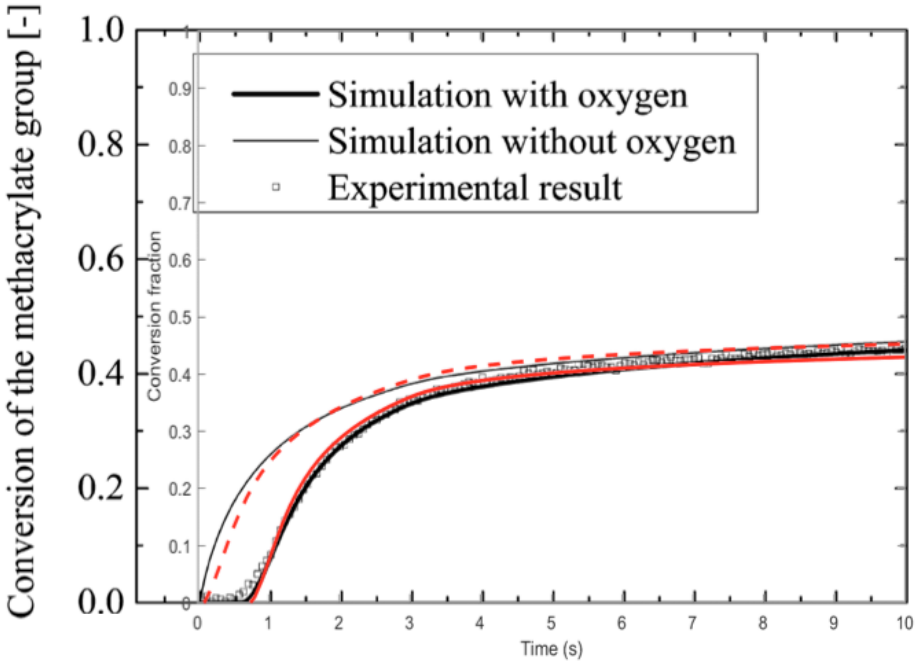
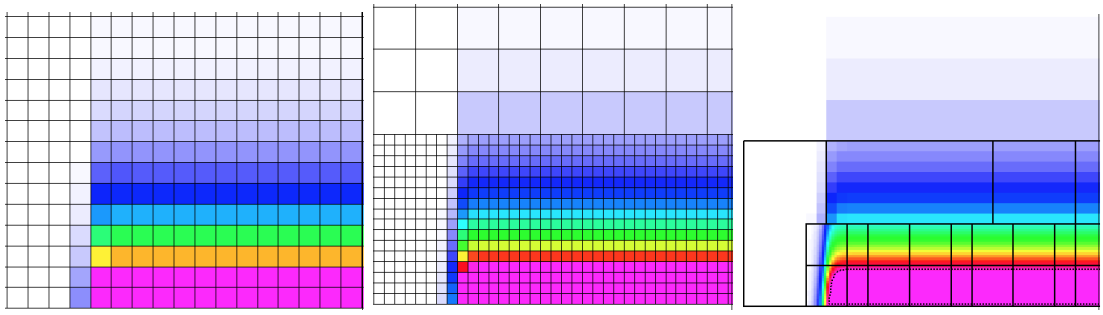


Figure 2: *Comparison of C++ code chemistry module with theory/experiment, when CLIP reaction chemistry begins to convert the resin into a solid. Red lines are HPC4Mfg C++ code results, compared to black lines and experiments in (Taki et al.).*.

2. "Dot" test: In a quiescent fluid, we add a local light source emanating from a "window" region at the bottom of the domain. The resulting reaction results in a "dot" of polymerized material which sits on the domain bottom atop the window itself, since there is no oxygen flow to create a dead zone. We had reasonable agreement between our final (steady-state) solution and Carbon's observations. Results of this test are shown in Figure 3, demonstrating the effectiveness of AMR at resolving the sharp concentration gradients produced by the combination of photochemistry and species transport.
3. "Dead-zone" test: Builds on the first test by adding an oxygen flux through the bottom boundary, which produces a dead zone where the reaction is inhibited. We were able to match Carbon's experimental results, with a 10um dead zone appearing at simulation resolutions of 1-2 um. Results of this test are in Figure 4.
4. "Part test 0": A simple rectangular part geometry with a constant draw velocity along with a matching light source is integrated to a steady-state in which the part withdrawal balances the polymerization rate at the bottom of the part. This tests the coupling between all three components of the model -- fluid flow, species transport, and reaction chemistry. We were still in the process of validating this test when the phase 1 project ended. Preliminary results were promising, as shown in Figure 5.



(a) (b) (c)

Figure 3: *Three different results from the O_2 diffusion-reaction "dot" test: (a) uniform 50 μm grid spacing, without AMR, (b) 1 level of 25 μm AMR from a coarser base, and (c) 2 levels of 4x refinement to a 6 μm grid spacing. At this finest resolution, the effects of oxygen diffusion can begin to be seen; the dotted contour line of the oxygen depletion zone has a radius of ~30 μm.*

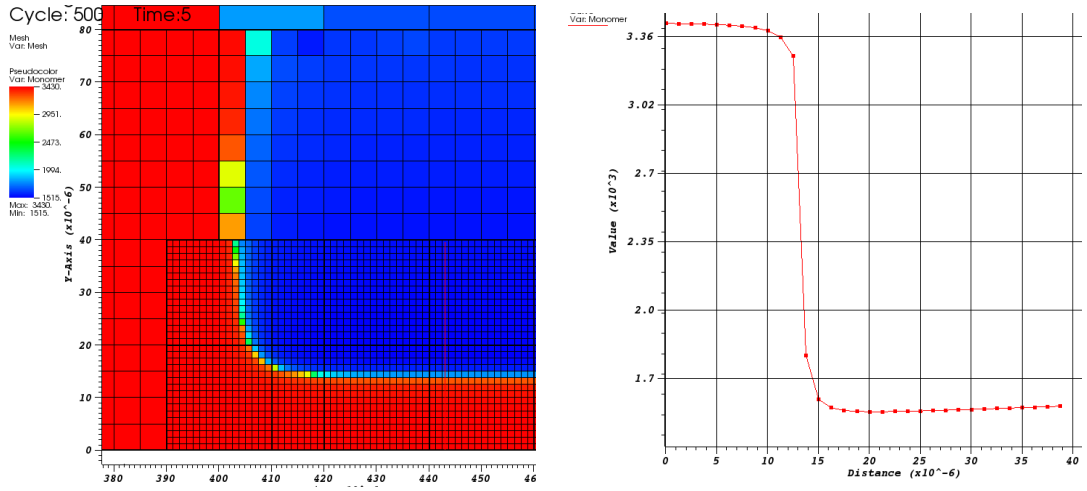


Figure 4: *"Dead-zone" test (a) showing the monomer concentration near the bottom boundary, where oxygen diffusion sustains a 10 um zone where (b) the reaction is inhibited and above which monomer is depleted.*

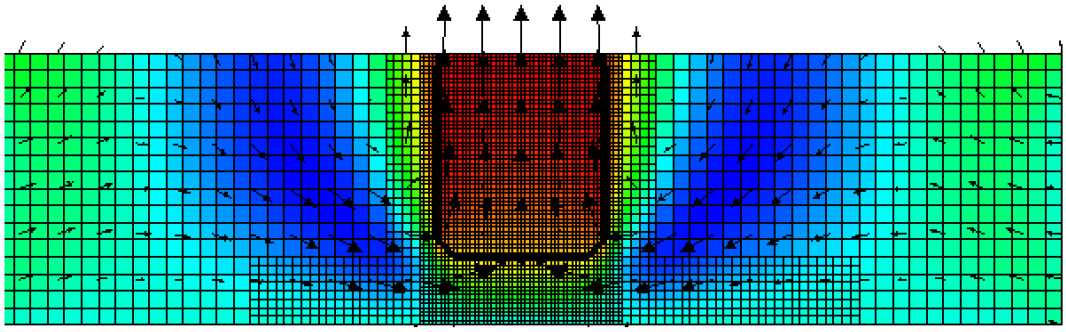


Figure 5: *Flow field induced around the part in the part withdrawal test, showing outline of part (black line), refined mesh around the part, and velocity induced by part withdrawal*

and polymerization at lower edge of the part. Colormap shows vertical velocity, while arrows show velocity field.

Discussion:
Due to a combination of stiffer-than-expected physics and a less robust than expected EB fluid-solver capability, this project became more of a development effort than originally planned. In particular, all three parts of the project required more development than originally expected: (a) the EB fluid solver initially planned for use in this effort was replaced by a solver which uses Brinkman penalization schemes to enforce the flow boundary conditions at the part boundary (b) due to stiffness in the O2 diffusion terms, we adopted a higher-order implicit-explicit (ImEx) scheme for advection-diffusion terms, and (c) stiffness in the photochemistry system took some time to diagnose and remedy.

As a result, we didn't fully accomplish our goals for this project, but the development accomplishments in this effort were substantial, and the test results indicate that the end result is very close to the useful process-modeling capability in the original proposal. We expect that with the basic pieces in place, further development will be much more rapid.

Also, because we were only beginning to bring the full capability online, we didn't use much of the HPC resources at our disposal. We leave that for a follow-on effort.

Summary:
A coupled fluid-species transport-photochemistry capability was developed to model the Carbon CLIP process. Due to technical complications in the model development process, the full modeling capability was not fully tested and validated; however, preliminary testing results are promising.

Implementation:
The software developed in this project was implemented using the FASTMath-supported Chombo C++ framework. All software has been delivered to Carbon, along with documentation.

Future work:
There is still work which can be done on the LBNL side to better meet Carbon's modeling needs, much of which will occur due to other ongoing Chombo development efforts:

LBNL expects the in-development EB fluid solver to come online soon, which would better match Carbon's model requirements. When that happens, we will contact Carbon to offer the improved solver as an update to the current capability.

Full validation of the model against observations remains to be carried out.

LBNL also plans to support the existing hand-off code with bugfixes and performance and capability improvements when relevant.

LBNL will write up the algorithm developed for this work in a general way which exposes no Carbon proprietary information, and will submit for publication after approval by Carbon.

Carbon expects to use the HPC4Mfg-developed code as a part of an enhanced in-house modeling effort.

References:

Q. Zhang, H. Johansen, and P. Colella, (2012) A Fourth-Order Accurate Finite-Volume Method with Structured Adaptive Mesh Refinement for Solving the Advection-Diffusion Equation, *SIAM Journal on Scientific Computing* 34 (2), B179-B201 https://doi.org/10.1137/110820105

Taki, et al, (2014) "Effect of Oxygen Inhibition on the Kinetic Constants of the UV-Radical Photopolymerization of Diurethane Dimethacrylate/Photoinitiator Systems," *Macromolecules*, 47, 1906−1913, dx.doi.org/10.1021/ma402437q