Complex Fluids Design Consortium (CFDC) at the University of California, Santa Barbara

Principles, Policies, and Operation

(Version April 19, 2017)

Executive Summary

The Complex Fluids Design Consortium (CFDC) is a consortium affiliated with the Materials Research Laboratory within the College of Engineering at the University of California, Santa Barbara (UCSB). The consortium enables a research partnership between computational fluids and materials scientists at UCSB and companies and national laboratories interested in the development of software tools for the design and behavior of complex fluids and soft material systems. A specific focus is the development of software tools built around statistical field theory models of complex fluid systems and the application of such tools to solution-borne formulations (e.g. personal care products), multiphase systems, and multi-component polymer alloys. The software design tools will connect composition and molecular architecture variables to self-assembly and structure, as well as address the dynamics, processing behavior and physical properties of such complex fluid mixtures.

Administration

CFDC is housed within the College of Engineering at UCSB and affiliated with the Materials Research Laboratory (MRL). The operations of CFDC are overseen by a Director in consultation with a Steering Committee. The Director is Glenn H. Fredrickson, Professor of Chemical Engineering and Materials.

The CFDC Steering Committee assists the Director in setting research directions for CFDC that meet the collective interests of the participants. The Steering Committee shall consist of 2 UCSB faculty participants, and one representative from each Corporate, National Lab, and non-UCSB Academic Partner.

Participation

Participants fall into four categories:

- **UCSB Partners.** Participants from UCSB are further subdivided in three categories:
    - *Faculty*, currently
        - Glenn H. Fredrickson, Professor of Chemical Engineering and Materials
        - L. Gary Leal, Professor of Chemical Engineering and Materials

        - Hector D. Ceniceros, Professor of Mathematics
        - Carlos Garcia-Cervera, Professor of Mathematics
    - *Postdocs*
    - *PhD students*
- **Non-UCSB Academic Partners.** Currently
    - Dr. Andrei Gusev**,** Department of Materials, ETH Zurich
    - Prof. Eric Cochran, Department of Chemical Engineering, Iowa State University
- **Corporate Partners.** Currently
    - Royal DSM
    - Intel
    - Dow Chemical
    - Asahi Kasei
    - JSR
    - SK Hynix
- **National Laboratory Partners.** The following laboratories and individuals are participating in CFDC:
    - *Los Alamos National Laboratory (LANL)*
        - Dr. Tony Redondo
        - Dr. Kim Rassmussen
    - *Sandia National Laboratory (SNL)*
        - Dr. John Curro
        - Dr. Amalie Frishknecht

Corporate and National Laboratory partners of CFDC are free to send any number of employees or representatives to participate in the programs of the CFDC. It is expected that CFDC-supported postdocs and PhD students may spend significant periods of time on site at partner locations.

Participation Level

Corporate Partners are expected to provide financial support in the form of an unrestricted cash gift or research contract to support the research activities of the center. There are three tiers of participation:

- **Sustaining Membership.** Membership at this level requires a minimum contribution of $35,000 per year in the form of an *unrestricted* gift or grant. In return, the partner can send any number of representatives to CFDC events, will receive software distributions, will be provided access to students and postdocs, and will be allocated one seat on the Steering Committee. Through this representation on the Steering Committee, the Partner will be able to influence group project definition and selection.
- **Intern Membership.** Companies or laboratories that wish to send an employee for an internship in the CFDC at UCSB will contribute $50,000 per year in the form of an *unrestricted* gift or grant to secure an Intern Membership. In addition to the benefits afforded Sustaining Members, Intern Members are able to

participate in a research project conducted by their designate employee intern at UCSB that is tailored to their specific interests. The intern will be provided a desk, library resources, and computer resources by the CFDC. The intern's salary and other expenses will be paid by the sponsor.

- **Full Membership.** Membership at this level requires a commitment to fund the entire cost of a graduate student or postdoctoral researcher through either an unrestricted gift (or grant) or research agreement (contract). In the case of a research agreement, funds will be subject to indirect cost recovery (overhead) by UCSB, but project objectives and intellectual property provisions can be defined. Current annual contributions to fund a PhD student or postdoc on an unrestricted gift are $60,000 and $80,000, respectively. Corresponding contribution levels to support a student or postdoc on a research contract (including UCSB overhead) are $90,000 and $120,000, respectively. In addition to the benefits afforded Sustaining Members, Full Members can participate in defining a research project to be executed by the student or postdoc that is tailored to their own R&D interests and objectives.

Full members are *strongly* encouraged to provide support in the form of an unrestricted gift. This mechanism lowers the overall cost of the project and avoids lengthy and often difficult negotiations to secure a research agreement.

Membership is granted with the expectation that a prospective Partner will participate for a minimum of two years. Subject to approval by the Steering Committee, up to 50% of a Partner's annual contribution can be in the form of in kind computing equipment or access to computing resources. National Lab Partners will contribute access to computational facilities and personnel time to participate in research projects and/or co-advise postdocs and graduate students. We expect that students and postdocs associated with the Consortium will spend significant amounts of time at Corporate and National Lab Partner locations.

Intellectual Property

The CFDC will endeavor to foster free and open communication among all participants with regard to the best tools and practices for molecular, mesoscopic, and macroscopic modeling of complex fluids, soft materials and multiphase systems. Specifically,

- Source codes of all software developed exclusively under CFDC will be distributed royalty-free to Corporate Partners upon request.
- Software distributions will be made according to the CFDC Software Distribution Policy appended to this document, which stipulates that software use is restricted to *non-commercial research and educational purposes*. Non-commercial use may include using the software for internal research and development purposes to identify or develop new materials or fluid-based formulations.
- Publications will be encouraged.
- The CFDC will respect intellectual property and other contractual obligations stipulated in a research agreement between UCSB and an individual Consortium

Member. UCSB will not engage in a research agreement that would render such obligations inconsistent with the principles and policies of the CFDC.

Scientific Programs

The design and optimization of complex and multiphase fluid formulations, such as oil/water emulsions, personal care products, plastic alloys, and processed foods, are difficult because of the presence of many components and often many coexisting phases. Exploration of the huge parameter space of such formulations by means of experiment or atomistic computer simulations is typically prohibitively expensive. Statistical field theory models that are coarse-grained to the *mesoscale* (atomic details below 1nm are removed) are particularly promising for analyzing the structure and thermodynamic properties of these types of complex fluids. Numerical methods to solve such models, i.e. to perform "field-theoretic computer simulations," are in a very early stage of development. If these methods can be made robust and efficient, and if the relevant interaction parameters can be deduced by experiment or atomistic simulations, "computational-combinatorial" exploration of the large parameter spaces that characterize complex fluid formulations could be carried out. Such an approach for examining the equilibrium phase diagrams and properties of structured soft materials is a major emphasis of the CFDC and would represent a paradigm shift in formulations design.

A second but related focus area of CFDC is on the *dynamics and processing* of such multiphase complex fluid systems. Of particular interest will be the development of computational methods that can handle geometrically complex multiphase structures within complex fluids, including phase separation in multi-component mixtures, droplet and bicontinuous emulsions, and formation of gas hydrates. Such approaches will be used to deduce fundamental insights into the relationship between flow and microstructure.

A third research focus area of CFDC will be to develop and integrate "property engines" for relating microstucture to physical properties. The design of soft materials involves not only an understanding of the relationship between molecular architecture and composition of the formulation with its equilibrium or non-equilibrium self-assembly, but also an understanding of the relationship between the self-assembled structure in a material and its liquid or solid state properties. Projects will be developed in CFDC to interface the output structures from mesoscopic simulations with finite element software packages that estimate properties ranging from elastic modulus to thermal conductivity to optical properties.

It is anticipated that the scientific directions and goals of the CFDC will evolve over time as Partners change, as previous objectives are met, and as the computational tools and methods advance. The Steering Committee will work with the Director to maintain clear directions for the Consortium.

Other Consortium Activities

Besides maintaining a set of collaborative research projects, the CFDC will sponsor other activities. Consortium Review meetings will be held at least once per year to disseminate research results, at which time the Steering Committee will also meet. Workshops, conferences, and other scientific gatherings will also be held periodically, depending on the interests of the Partners. Events to foster interactions and employment opportunities between CFDC-supported students and postdocs and the Corporate and National Lab Partners are also envisioned.

Software Distribution Policy

Complex Fluids Design Consortium (CFDC)
University of California at Santa Barbara (UCSB)

It is the policy of the Complex Fluids Design Consortium to provide consortium members access to computer software (including source codes) first developed with Consortium funding for *non-commercial research and educational purposes* at no cost whenever possible. Non-commercial use may include using the software for research and development purposes to identify or develop new materials or fluid-based formulations. Consortium members may request a letter confirming the availability of a no-cost non-commercial license for a particular piece of software that will contain the following indemnification clause:

"Recipient acknowledges and agrees that the software shall be provided "as is," and, as such, the University MAKES NO REPRESENTATIONS AND EXTENDS NO WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED. THERE ARE NO EXPRESS OR IMPLIED WARRANTIES OF MERCHANTABILITY OR FITNESS FOR A PARTICULAR PURPOSE. The University will not be liable to Recipient for any loss, claim or demand made by Recipient, or made against Recipient by any other party, due to or arising from the use of the software by Recipient. This letter does not: (a) express or imply a warranty or representation as to the validity or scope of any of the Regent's intellectual property rights; (b) express or imply a warranty or representation that anything made, used, sold, offered for sale or imported or otherwise disposed of under any license granted in this Agreement is or will be free from infringement of the intellectual property rights of third parties; (c) obligate the Regents to bring or prosecute actions or suits against third parties for intellectual property infringement; (d) confer by implication, estoppel or otherwise any license or rights under any intellectual property rights of the Regents other than the rights as expressly granted herein; or, (e) obligate the Regents to furnish any know-how except for such know-how the University expressly agrees to provide through this Agreement."

Should a company desire access to Consortium-developed software for commercial purposes, it should contact Prof. Glenn Fredrickson, Director of CFDC.