PIRE Project at City College of New York (2017-2022)

Multi-scale, Multi-phase Phenomena in Complex Fluids for the Energy Industries

Masahiro Kawaji
Professor of Mechanical Engineering
City College of New York
Acting Director, The CUNY Energy Institute

- NSF - Partnerships for International Research and Education (PIRE) Grant
  - Funding: $5.2 million
  - Duration: 5 years
- U.S. and foreign sponsors

  US – National Science Foundation, Office of International Science & Engineering

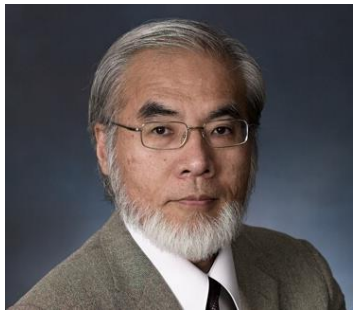
  Norway – Research Council of Norway (RCN)

  France – Agence Nationale de la Recherche (ANR)

  Germany - Deutsche Forschungsgemeinschaft (DFG)

Participants from City College of New York

PI: Masahiro Kawaji (Prof. of Mechanical Engineering; Acting Director, CUNY Energy Institute)



Co-PI: Sanjoy Banerjee (Distinguished Prof. of Chem. Eng.; Director, CUNY Energy Institute)

Co-PI: Robert Messinger (Asst. Prof. of Chemical Engineering; CUNY Energy Institute)

Co-PI: Jeff Morris (Prof. of Chemical Engineering; Director, Levich Institute)

Co-PI: Vincent Pauchard (Assoc. Prof. of Chemical Engineering; CUNY Energy Institute)

Senior Personnel: Taehun Lee (Assoc. Prof. of Mechanical Engineering; CUNY Energy Institute)

Senior Personnel: Joel Koplik (Prof. of Physics; Levich Institute)

Senior Personnel: Charles Watkins (Prof. of Mechanical Engineering)

Acknowledgements

- Mr. John Tsapogas
  - Director, Office of Award Pre-Proposal Support, RF CUNY
- Ms. Keiko Sometani
  - Grants and Sponsored Programs, CCNY
- Ms. Anna Volovik
  - PIRE Project Coordinator, CCNY

Norwegian collaborators

Norwegian Foundation for Scientific & Industrial Research (SINTEF)

Harald Linga (Research Director, Petroleum Research)

Bjornar Lund (Senior Scientist, Dept. of Multiphase Flow)

Roar Larsen (Chief Scientist)

Martin Fossen (Research Scientist, Dept. of Multiphase Flow)

Norwegian University of Science and Technology (NTNU)

Ole Jørgen Nydal (Prof. of Energy and Process Engineering)

Sigbjørn Sangesland (Prof. of Petroleum Engineering and Applied Geophysics)

Pål Skalle (Prof. of Geoscience and Petroleum)

University of Oslo (UIO)

Atle Jensen (Prof. of Mechanics, Leader of Hydrodynamics Laboratory)

Andrea Carlson (Assoc.Prof., Depts. of Mathematics & Mechanics)

French collaborators

National Polytechnic Institute of Toulouse (INP-ENSIACET)

Olivier Masbernat (Prof. and Director of Research, Chemical Engineering Laboratory)

Micheline Abbas (Associate Prof., Chemical Engineering Laboratory)

National Research Institute of Science & Technology for Environment & Agriculture (IRSTEA)

Laurence Fournaison (Head, Refrigerating Process Research)

Anthony Delahaye (Head, Refrigeration Systems Group)

École Nationale Supérieure de Techniques Avancées (ENSTA ParisTech)

Didier Dalmazzone (Prof. of Chemical Engineering)

Laboratoire de Chimie et Physique Quantiques (LCPQ)

Aude Simon (CNRS Research Scientist)

German collaborators

Karlsruhe Institute of Technology (KIT)

Mathias J. Krause (Inst. for Applied and Numerical Mathematics)

University of Hamburg (UH)

Philipp Neumann (Department of Informatics)

Ruhr-Universität Bochum (RUB)/Fraunhofer UMSICHT

Goerge Deerberg (Inst. for Thermo & Fluid Dynamics)

Fraunhofer ISE

Stefan Gschwander (Heat and Cold Storages Group)

Peter Schossig (Heating and Cooling Tech. Dept.)

Leibniz Institut für Polymerforschung Dresden e.V. (IPF)

Ulrich Scheler (Polyelectrolytes & Dispersions Dept.)

PIRE Project at City College of New York (2017-2022)

VISION

- Acceleration of research, education and training in multi-phase fluid engineering science
- Development of a diverse STEM workforce by creating an international collaborative network with advanced research tools

OBJECTIVES

1. To advance knowledge and make transformative scientific discoveries to improve energy and process efficiency in industrial systems on a global scale.
2. To accelerate education and training of students and postdocs by providing unique opportunities in international research
3. To build strong international partnerships by sharing resources and research infrastructure within and across institutions

Research Problem

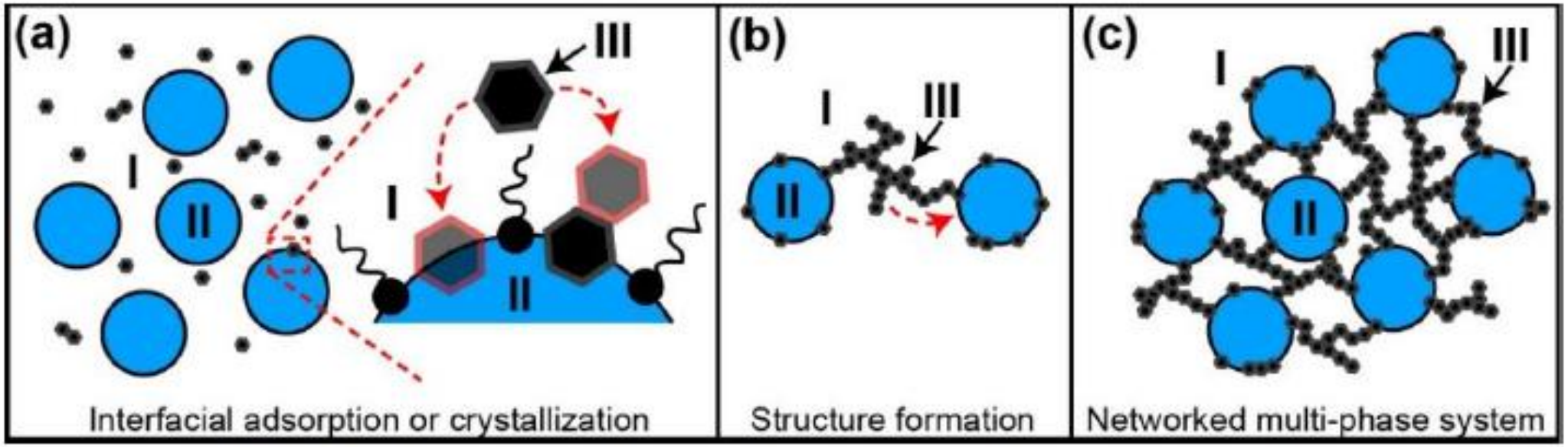


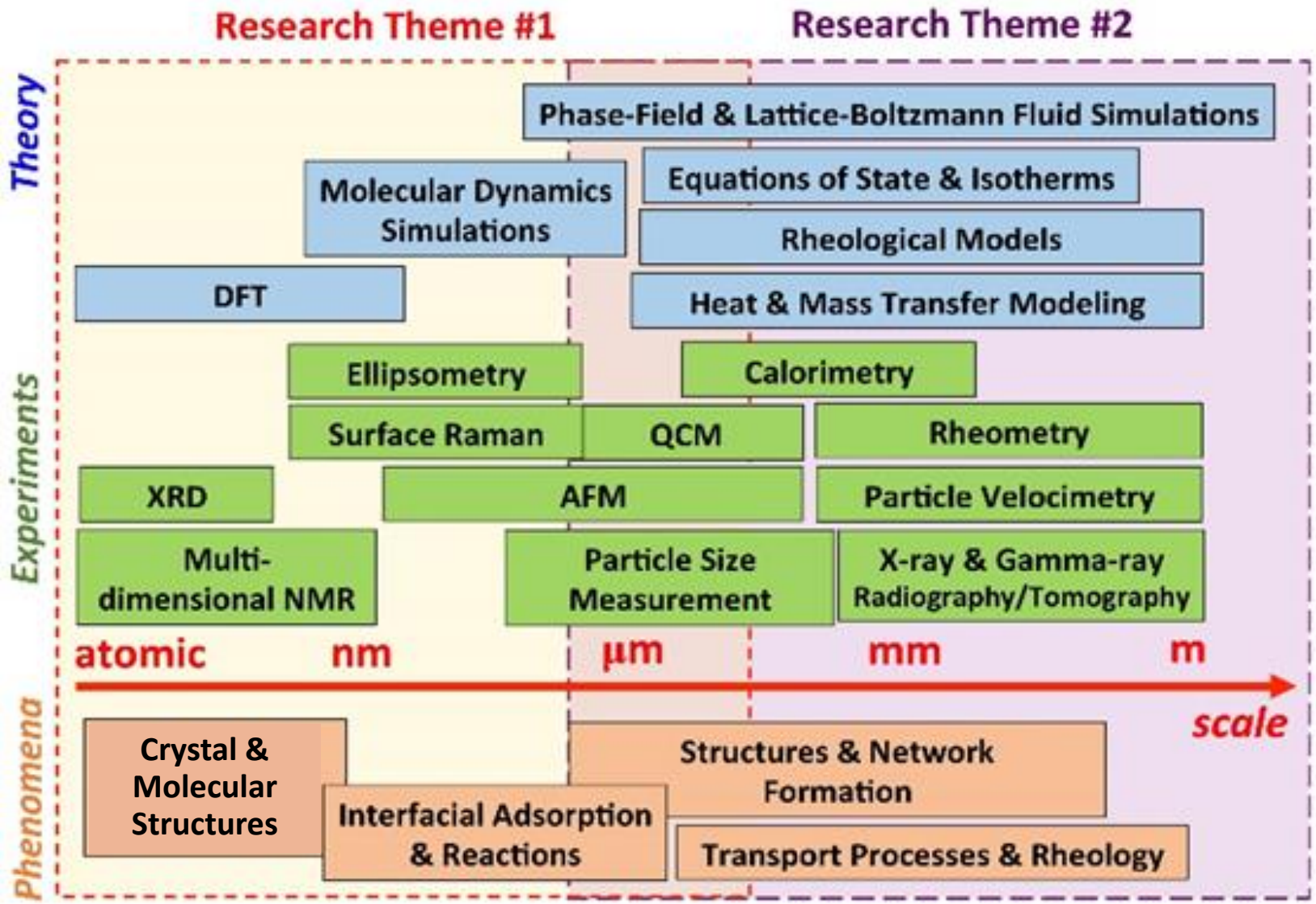
Fig. 2 Schematic of the multi-scale, multi-phase problem.

A continuous liquid phase (I)
An internal phase (II) dispersed in (I) i.e., an emulsion of droplets or dispersion of solid particles
Molecular species, aggregates, or particles of a network-forming phase (III)

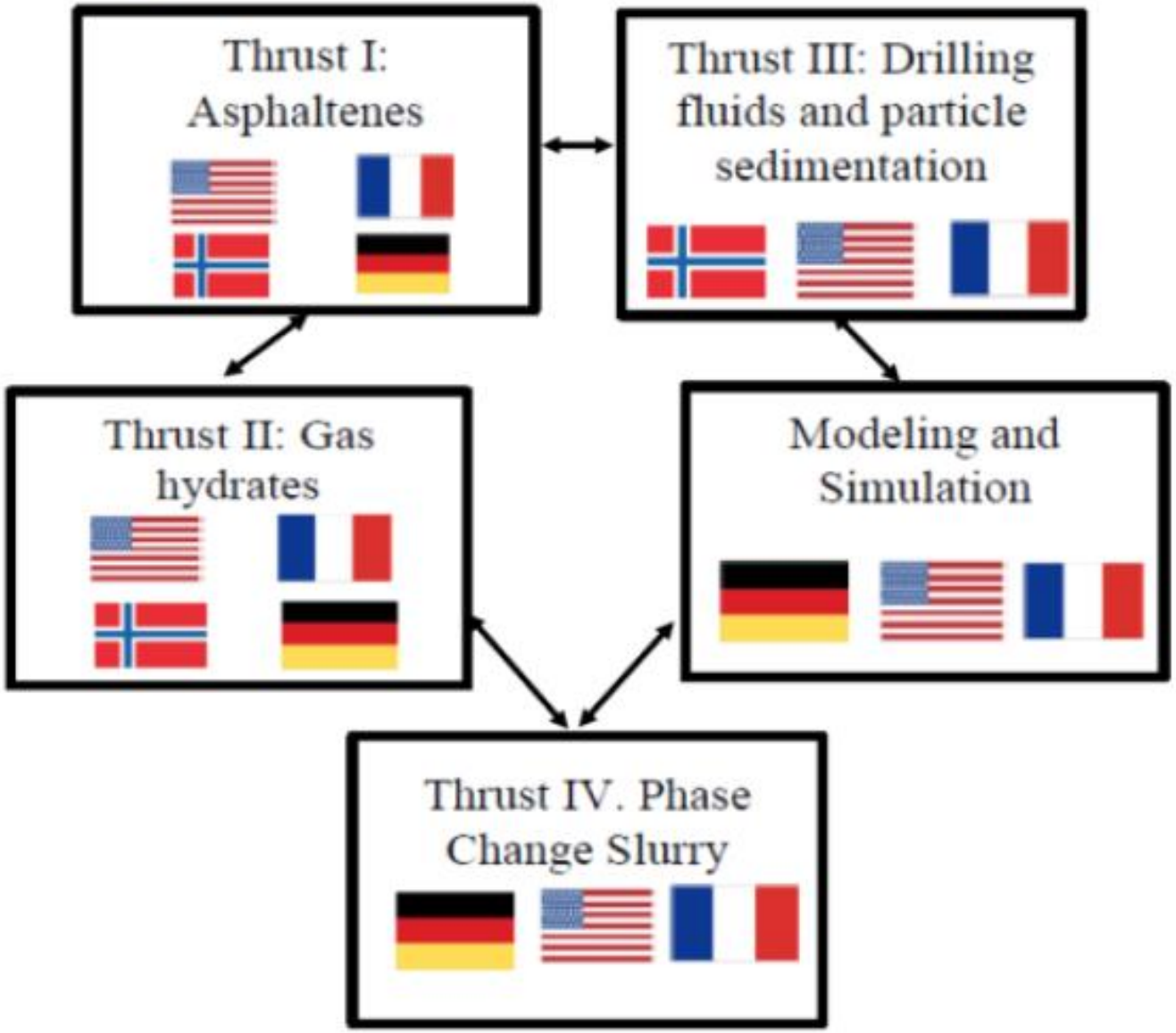
Research Theme #1. Molecular-scale phenomena in complex, multi-phase fluids

Research Theme #2. Macroscopic complex fluid transport processes and properties

Multi-Scale Research Themes



Research Thrusts



Research Thrusts

Experimental Research Thrusts

I. Asphaltene Adsorption, Aggregation, and Interfacial Effects

(CCNY: Pauchard, Banerjee, Messinger, Koplik, Lee; SINTEF: Fossen, Larsen, INP-LGC: Masbernat, LCPQ: Simon; IPF: Scheler)

II. Formation and Control of Gas Hydrate Slurries

(CCNY: Morris, Pauchard, Kawaji, Banerjee, Messinger, Lee; IRSTEA: Fournaison, Delahaye; ENSTA ParisTech: Dalmazzone; RUB/Fraunhofer UMSICHT: Deerberg, Janicki; SINTEF: Fossen, Larsen)

III. Drilling Fluids and Mechanisms of Particle Sedimentation

(CCNY: Banerjee, Kawaji, Morris; SINTEF: Linga, Lund, Larsen, Fossen; NTNU: Nydal, Sangesland, Skalle; UIO: Jensen, Carlson; INP-LGC: Masbernat, Abbas)

IV. Phase-Change-Material Nanoemulsions for Energy Transport and Storage

(CCNY: Kawaji, Messinger; Fraunhofer ISE: Gschwander, Schossig; IRSTEA: Delahaye, Fournaison; ENSTA ParisTech: Dalmazzone; INP-LGC: Masbernat; IPF: Scheler)

Modeling and Simulation

- Quantum ab initio simulations, Classical molecular dynamics (MD), Random Sequential Adsorption (RSA), Lattice Boltzmann Method (LBM), Discrete Element Method (DEM)

Building on Prior Collaborations

- France
  - M. Kawaji was a visiting scientist at IRSTEA in Paris (2006)
  - J. Morris is Chair d'Attractivite, FERMAT Foundation (Univ. of Toulouse) 2015-2019
- Norway
  - S. Banerjee was a member of the Norwegian Gov't – Industry Board on Flow Assurance (FACE) 2008-15
  - V. Pauchard was a project leader of the Flow Assurance Center of Innovation at SINTEF, 2009-2014, before coming to CCNY
- Germany
  - T. Lee had recently started collaborating with KIT
  - R. Messinger knew Scheler at Leibniz Institut, Dresden
- Common research interests and complementary expertise and facilities would lead to synergy and strengthening of our research competitiveness
  - Norway can provide real samples of drilling fluids and crude oil
  - France has a CO_2 hydrates test facility and modeling capability
  - Germany offers unique computational and experimental resources

Table 1. Past and Proposed Collaborations with International Partners.

(Research Thrust 1: Asphaltenes; Thrust 2: Gas Hydrates; Thrust 3: Drilling Fluids; Thrust 4: PCM Nanoemulsion)

Country	Partner Institutions	Past Collaborations with CCNY	Research Areas for Collaboration	Unique Strengths of the Partner
Norway	SINTEF	R&D program FACE in 2007-14: Topics on droplet coalescence and separation, modelling and experiments.	Thrusts I and III	Large scale, high pressure/temp. studies of non-Newtonian fluids and drilling fluids. Network of industry and academia.
	NTNU			Multiphase flow: experiments and modelling.
	UiO			High resolution measurement of flow field.
France	IRSTEA/ ENSTA Paris Tech	Phase change slurry, ice slurry, modeling of ice slurry melting.	Thrusts II and IV	Extensive experience in CO_2 hydrate slurry, measurement and modeling tools for system characterization. Research quality, Facility
	INP-ENSIACET	Thermodynamics and stability of water-crude oil interfaces in FACE.	Thrusts II, III, IV	Expertise in dense emulsions, simulations of suspensions and interface rheology; Crystallization kinetics; Self-assembly.
	LCPQ	Modeling the asphaltene solution at water interface, quantum effects (started in 2016)	Thrust I	Ab initio molecular dynamics simulations, expertise in DFTB electronic structure method, developments and applications within an open source code, computer resources.
Germany	KIT	Particulate Fluid Flow Simulations.	Modeling and Simulation	Open Source Software "OpenLB" for simulation of complex fluid flows.
	RUB Fraunhofer UMSICHT	None	Thrust II	Extensive analytical tools, mathematical models and simulation software for thermodynamics, kinetics, physical properties of hydrate based processes and for process development.
	Fraunhofer ISE	None	Thrust IV	Thermal Characterization of PCMs, Test facilities and extensive knowledge of PCM nanoemulsion properties.
	IPF	Rheo-NMR measurements.	Thrusts I and IV	Rheo-NMR, PFG-NMR, Developing new NMR apparati.

Country	Partner institutions	Perceived Mutual Gains from the Partnership	No. of Researchers	No. of Grad. Students	Provider of Financial or In-Kind Support
Norway	SINTEF	Strengthening R&D offerings and capabilities towards the oil & gas industry. Share R&D results on related fluid transport issues with partner institutes.	4	3	Research Council of Norway (RCN): 5 Million NOK/year (577,000 USD/year) for 5 years.
	NTNU	Access to complimentary data on surface effects in particle-non-Newtonian fluid systems and model concepts.	3	2	
	University of Oslo (UiO)	Experimental set-up and methodologies for high resolution flow field studies of model systems, as extended to non-Newtonian fluids and particle settling.	2	2	
France	IRSTEA/ ENSTA Paris Tech	PhD students, sharing of measurement and modeling tools, increase the international partnership on complementary research. Interaction with other fields of application for hydrates and slurries.	4	1	In-kind: 18 months of PhD student (shared with ENSTA), 32 months of researchers
	INP-ENSIACET	Enhancement of expertise in complex flow/interface modeling, thermodynamics/rheology, dedicated instrumented experiments that will be reused in future/collaborative network.	5 researchers + 2 research engineers	3 potdocs + 0.5PhD	University of Toulouse INPT; CNRS; ANR
	LCPQ	New significant applications of our methodology, extension and sharing of our knowledge, increase of our visibility abroad, interaction with other fields, exchange of PhD students.	2	1 or 2	CNRS, University of Toulouse
Germany	KIT	Building a strong community on Complex Flow Simulations, Sharing software development resources, Sharing results to develop Sustainable Models/ Software.	2	8	DFG: KIT will request 320k Euro for 2 PhD students and travel
	RUB/ Fraunhofer UMSICHT	Scientific exchange of knowledge, Support of joint developments, Fundamentals related to gas hydrates and adsorption of gases on porous media (experimental and numerical), Strengthening the domains of excellence, - Cross-disciplinary research	2	1	DFG/Institutional support
	Fraunhofer ISE	Exchange of scientists and PhD students.	2	TBD	Institutional support
	IPF	CCNY: Access to unique NMR methods.	1	1	DFG: IPF will request 150k Euro/year

Funding Status for Foreign Collaborators

Country, Funding Agency	Institution	Application status	Funding level	Duration
Norway and NRC	SINTEFF NTNU University of Oslo	Submitted and partially approved	1.15 million USD approved to date out of 3.13 million requested	5 years
Germany and DFG	Leibniz-Institut, Dresden	Submitted and decision expected in December, 2017	Stipend for one PhD student	3 years
	Fraunhofer - UMSICHT		310,000 Euros	3 years
	University of Hamburg		400,000 Euros	3 years
	KIT			
France and ANR	IRSTEA ENSTA- ParisTech INP-ENSIACET LCPQ	Submitted on October 26	550,000 ~ 600,000 Euros	3.5 years

Educational Goals

- To mentor and train outstanding undergraduate and graduate students, and postdoctoral researchers at CCNY, and contribute to the development of the STEM workforce
- Recruit UG, Master's and PhD students from underrepresented groups
- To provide undergraduate and high school students with opportunities for research experience and interactions with foreign collaborators

Educational Aspects

- **Diversity:** 7 PhD students, 3 postdoctoral fellows, 10 Master's students and 10 undergraduate students will be recruited and supported, many from underrepresented minority groups, including women.
- **Recruitment**: Aggressive recruitment including an annual weekend program for undergraduate and Master's students.
- **LSAMP** will fund two CUNY underrepresented-minority undergraduate scholars for summer research experiences at our international partner institutions.
- **Mentoring**: PIRE faculty and collaborators will mentor students and enable them to work in the state-of-the-art research facilities (e.g., ASRC) at CCNY and international partners.
- **Foreign Experience:**
  - Attendance at Annual Review Meetings in NYC, Norway, France, and Germany
  - 6 month-long Internships for PhD students and summer internships for UG students at partner institutions
  - Visits to partner institutions
- Industrial perspectives will be provided by SINTEF in Norway, IRSTEA in France and Fraunhofer Institute in Germany.

Foreign Experience

Overseas Trips by PhD students *V: Research Visits, INT**: 6-month** Research Internships, & ARM: Annual Review Meetings*					
PhD Students	**Year 1**	**Year 2**	**Year 3**	**Year 4**	**Year 5**
#1	V	INT + ARM	ARM	V + ARM	
#2	V	INT + ARM	ARM	V + ARM	
#3	V	INT + ARM	ARM	V + ARM	
#4		V + ARM	INT + ARM	ARM	V
#5		V + ARM	INT + ARM	ARM	V
#6		V + ARM	ARM	INT + ARM	V
#7		V + ARM	ARM	INT + ARM	V

Training on Advanced Research Tools:

- Multi-dimensional NMR spectroscopy at CCNY
- FBRM and capillary rheometry at IRSTEA
- High pressure rheometry and *in situ* FTIR at ENSTA ParisTech
- X-ray and gamma-ray techniques at CCNY and University of Oslo
- DSC and Rheometry at IRSTEA, ENSTA Paris, Fraunhofer ISE and CCNY
- Rheo-NMR & PFG-NMR at IPF Dresden
- Lattice-Boltzmann simulations at CCNY, KIT, HB, and MD at CCNY and ENSTA ParisTech
- Rheometry and flow modeling at CCNY, Fraunhofer UMSICHT and ISE
- Pendant droplet and QCM at CCNY and SINTEF
- DFT at CNRS
- High pressure µDSC, calorimetry, gravimetric analysis, density and thermal conductivity measurements at RUB/Fraunhofer UMSICHT

Outreach Activities

- Middle and High School Researcher Program: recruitment of high school students and teachers to experience research in CCNY labs of PIRE faculty
- Engineering Networking Reception will be attended by high school science teachers and community college professors
- Open houses with lab demonstrations and short seminars for Middle/High School students and General Public
- PIRE researchers will give seminars, serve as judges at local Science Fairs and organize Science Cafes

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News Release 17-085

NSF announces 14 new PIRE awards to support scientific collaboration in 24 countries

US researchers leverage international partnerships to extend the frontiers of science, engineering and education

Katrien Keune, European collaborator on the CuBISM PIRE project, analyzes a painting at Rijksmuseum. Credit and Larger Version

2017 PIRE Competition

- 254 preliminary proposals received (September 2016)
  - Number of engineering preliminary proposals submitted: 68

- 71 were invited to submit full proposals
- 14 Proposals selected for Funding
  - 5.5% of preliminary proposals and 20% of full proposals
- Average award size: $4,765,228
- Duration: all awards are for 5 years
- Number of engineering awards made: 3
  - 4.4% of preliminary engineering proposals

Suggestions for new PIRE Proposals

Factors for our successful PIRE proposal and best practices for creating strong international research and educational collaborations

- Solid track records by PIRE faculty in research and education
- Building on strong prior research collaborations
  - Additional collaborators identified and invited to participate in order to balance the number of researchers involved in different thrusts from partner countries
  - ➢ A truly multi-national collaboration and not a collection of bi-national collaborations
- Partner relationships are clearly defined and explained
  - Unique strengths and mutual benefits

Additional Suggestions for new PIRE Proposals

- Well planned Management structure, important for large projects with many participants
  - Appointment of a Project Coordinator
  - Advisory Board

- Well defined evaluation and assessment plan by an experienced evaluator

Management Structure

Advisory Board Members

Academia

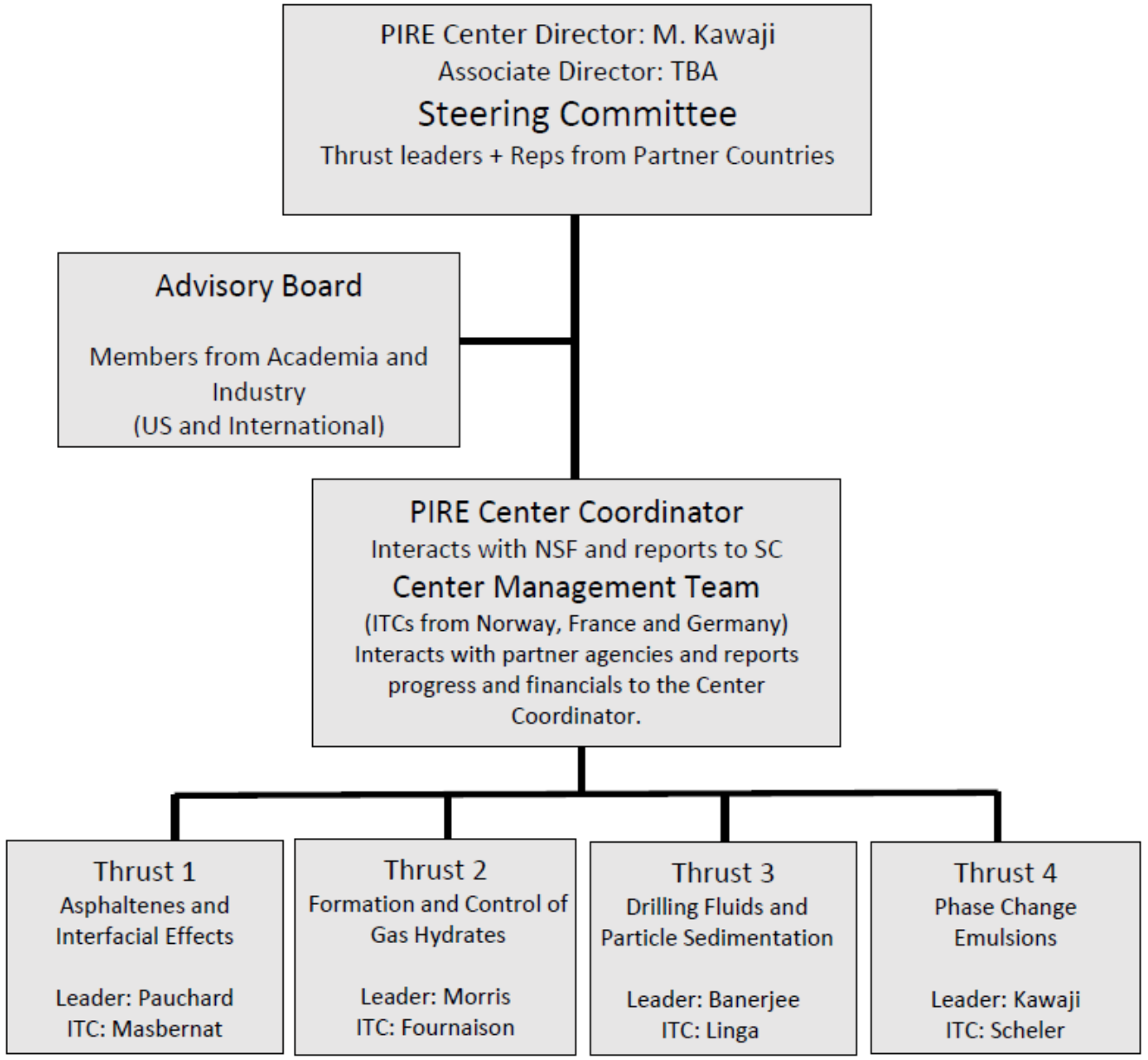
- L. Goual of U. Wyoming
- F. Vargas of Rice University
- M. Denn of CCNY

Industry

- H. Kallevik of Statoil (Norway)
- O. Mullins of Schlumberger

Engineering Societies

- One or more from minority organizations, NACME, GEM, LSAMP, SHPE, NSBE, and SWE



EVALUATION AND ASSESSMENT

- External evaluator: Dr. Denis Gray, Professor of NC State University
  - has 30 years experience in evaluation of NSF IUCRC program and serving as local evaluator of STC, IGERT, PIRE and other federal initiatives.
- Well-defined Evaluation and Assessment Criteria

1. Support excellence in STEM research and education through international collaboration
2. Promote international research and educational opportunities
3. Sharing of resources and research infrastructure with international partners
4. Students gain substantive international research experiences

Additional Suggestions for new PIRE Proposals

- Many months needed for proposal preparation
  - 20 pages of narrative + signed institutional letters of commitment and individual letters of commitment, CVs, Current and Pending, Conflict of interest, Data management plan, Facilities and resources, Prior NSF grants, etc.
- Extensive and timely communication with international collaborators
- Pre-submission review of a draft proposal by three external reviewers
- Submit the final proposal at least one day before the deadline
  - Uploading individual CV's one at a time (28 CVs in our case)
  - NSF's PIRE submission website was slow and sometimes down on the due date
  - Deadline was extended by 2 days

Thank you!