H1. FULL DESCRIPTION

1 Research Project Objectives

The subject of the project is sea ice dynamics, especially dynamics of strongly fragmented sea ice and processes leading to fragmentation, as well as sub-mesoscale interactions of the sea ice cover with the ocean and the atmosphere.

On the list of the project objectives, reference is made to the sea ice model called DESIgn (Discrete-Element bonded-particles Sea Ice model), which is going to be the main tool used to accomplish these objectives. It is described in further sections of this document.

The main project objectives are:

- To improve existing and to develop new mathematical models of sea ice–waves interactions suitable for further implementation in discrete-element bonded-particle models, i.e., consistent with basic underlying concepts and assumptions of these models.
- To formulate, based on the theoretical results, numerical ice–waves interaction algorithms, and to implement these algorithms in the code of the DESIgn sea ice model.
- To verify a hypothesis that: (i) wave-induced breaking tends to produce narrow floe-size distributions and polygonal floe shapes and (ii) that further "grinding" and diminution of ice floes by shearing deformation in the inner parts of the marginal ice zone is responsible for the widely observed heavy-tailed floe-size distributions and rounded floe shapes.
- To extend the range of applicability of the DESIgn model by developing and implementing parametrization schemes for selected physical processes (e.g., pressure ridging; freezing and melting). Also, to add new functionalities that will facilitate further development of the model, including time-variability of the properties of the model components (grains and bonds).
- To improve our understanding of processes and factors that may lead to rapid fragmentation and decomposition of the sea ice cover over large domains, similar to the dramatic break-up event that took place in the Beaufort Sea in winter 2013.
- To use high-resolution numerical modeling to improve our understanding of the atmosphere–sea ice– ocean interactions in situations with strongly fragmented sea ice and/or close to the ice edge. In particular, to analyze the influence of the floe-size distribution on heat and momentum fluxes at the sea surface, as well as on turbulence, mixing processes and vertical stability in the tropospheric and oceanic boundary layers. Also, to verify the existing hypotheses regarding mechanisms of ice-band formation close to the ice edge.
- To develop parameterizations of the above-mentioned effects, taking into account the floe-size distribution, suitable for future implementation in continuum sea ice models.

Taken together, the results of this project should contribute to the improvement of the performance of numerical sea ice models, especially in situations with strongly fragmented ice cover.

Moreover, the project will provide the sea ice community with a new, significantly improved version of a discrete-element sea ice model that – similarly to its present version – will be freely available to everyone to use and modify.

2 Significance of the project

2.1 State of the art and justification for the choice of scientific problems

The recent large-scale, hemispheric trends in sea ice extent are well known and hotly debated among professionals and the general public alike (Fig. 1). Whereas state-of-the-art climate models consistently predict a decline of the Arctic sea ice extent during the 21st century, the observed negative trend in the period in which observations are available (red line in the left panel of Fig. 1) is roughly three times faster than the ensemble mean of the models. Moreover, even when the models are analyzed separately, none of them is able to

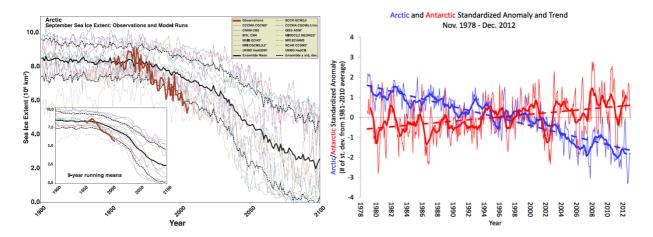


Figure 1: Variability and trends of sea ice extent. Left: Arctic September sea ice extent from observations (thick red line) and from 13 IPCC climate models. Solid and dashed black lines show the ensemble mean and ± 1 standard deviation, respectively (source: Stroeve et al. (2007)). Right: Observed Arctic and Antarctic sea ice extent anomalies in the period 1979–2012. Thin lines show the monthly anomalies, thick lines – the 12-month running means (source: National Snow and Ice Data Center, University of Colorado, Boulder; https://nsidc.org/cryosphere/sotc/sea_ice.html).

reproduce the observed trend value (Stroeve et al., 2007). This clearly suggests that some important physics is missing in the models and/or that the existing parametrizations do not capture the essential large-scale effects of processes they should account for. To make matters more complex, the observed trends of sea ice extent on the Southern Hemisphere, although slower, are not negative, but positive. The response of the sea ice cover to the global climate change is thus dependent on hemispheric and regional factors. A related, and largely unanswered question is how changes in sea ice extent are related to changes in sea ice volume, age (multiyear versus first-year ice) and sea ice properties like, e.g., its mechanical strength and thus response to oceanic and atmospheric forcing. Observations clearly show that the extent and thickness of multi-vear ice in the Arctic has been decreasing (see, e.g., Comiso, 2012). Many feedbacks are involved. Due to lower mechanical strength of the thinning ice, it gets more easily deformed and transported by winds and currents. For example, Rampal et al. (2009) showed that both the mean speed and the deformation rate of sea ice in the Arctic have increased since the 1980ies. A numerical study of inertial oscillations of sea ice (Gimbert et al., 2012) has led to the same conclusions. Stronger deformation rates of sea ice generally lead to the increase of the total sea ice volume in winter (due to increased new ice production in leads) and to the decrease of the total sea ice volume in the summer (due to increased lateral melting). Positive feedbacks between sea ice fragmentation and sea ice loss in the summer have been analyzed recently by Asplin et al. (2012, 2014), who pointed out that decreasing sea ice extent and the associated larger areas of open water lead to larger storm-induced waves, which can penetrate deeper into the weakening ice cover and lead to faster melting and even larger waves in subsequent storms (and in the polar regions the summer is the season with the strongest storms; see, e.g., Simmonds and Rudeva, 2012). Asplin et al. (2012) conclude their work that "this process will have implications for modeling future sea ice dynamics and thermodynamics, and needs to be included in regional and large scale climate models to enhance processes of sea ice decay, formation and motion".

On synoptic scales, state-of-the-art continuum sea ice models generally provide reliable results in terms of average, basin-scale sea ice concentration and velocity patterns, but they fail to reproduce statistical properties of sea ice deformation (Girard et al., 2009). In terms of the modeling of sea ice response to deformation, substantial progress has been made in recent years. For example, the elasto-brittle rheology proposed by Girard et al. (2011) and the Maxwell-elasto-brittle rheology of Dansereau et al. (2015) significantly improve the ability of large-scale sea ice models to produce realistic deformation patterns. Similarly, Wilchinsky and Feltham (2011) developed theoretical foundations and implemented an anisotropic sea ice rheology based on an assumed rhomboidal geometry of ice floes in order to model Coulombic failure of sea ice. New numerical-modeling techniques have been proposed as well, like for example the model by Rampal et al. (2015) based on the Lagrangian dynamics, which enables to preserve sharp boundaries and highly localized features in the ice cover (leads, pressure ridges etc.). Even though all these recent achievements bring us closer to reproducing the observed intermittent, localized, multifractal character of sea ice deformation (see, e.g., Marsan et al.,

2004; Weiss and Marsan, 2004; Hutchings et al., 2011; Herman and Glowacki, 2012), making the large-scale models both accurate and computationally efficient remains a challenge.

Limitations of the state-of-the-art large-scale sea ice models become visible during extreme deformation events, like the one that took place in the Beaufort Sea in February and March 2013. During a prolonged period of relatively strong and persistent winds from the east and northeast, dense cracks appeared in the sea ice cover north of Point Barrow, which subsequently propagated first to the northeast, and then to the east (Fig. 2), so that in early March the whole, 1.5-million-km²-area was covered with loose floes that could be easily transported by winds and currents towards the Bering Strait and out of the Arctic (a full animation of this break-up event can be found at http://earthobservatory.nasa.gov/IOTD/view.php?id=80752). Brittle nature of sea ice deformation during this time period can be clearly seen in Fig. 2. Notably, some systems of almost parallel cracks have lengths of over 500 km, resulting in extremely elongated floes; another important feature is a narrow zone close to the coast west and north of Point Barrow, where the ice was broken into very small floes (upper image in Fig. 2) due to compression and shear. The contribution of this area to the propagation of damage over the whole Beaufort Sea and the southwestward ice transport is hard to estimate without a model that would be able to reproduce all above-mentioned features of ice deformation. As similar events are likely to occur more frequently in the future, it is crucial to develop such models and to identify factors that may contribute to such rapid changes of the state of the sea ice cover. (It is worth noting that in this case, wind waves are an unlikely candidate for such a factor, as there was no open water in the Arctic at that time where wind waves could develop.)

A very important recent achievement is the formulation of prognostic equations for the joint ice-thickness and floe-size distribution, suitable for continuum sea ice models (Horvat and Tziperman, 2015). Whereas analogous equations for the ice-thickness distribution are well established and widely used since a couple of decades, there was no equivalent for the floe-size distribution until a few months ago. The importance of this milestone will become clear in the future, as more parametrizations of various floe-size dependent processes become available. The equations of Horvat and Tziperman (2015) provide a universal, consistent framework in which these new parametrizations can be directly incorporated.

After many years of relative stillstand, last years brought also a revival of interest in discrete-element sea ice models, not least thanks to the work of the Principal Investigator of this project, who used this approach to analyze the influence of the floe-size distribution on "herding" of ice floes on the sea surface, on the response of ice to shear deformation, and on the properties of force networks and jamming phase transition in various conditions (Herman, 2011, 2012, 2013b,c). A review of discrete-element and related methods in sea ice modeling can be found in Herman (2015). The most recent work in which this approach is used is by Rabatel et al. (2015).

In terms of our ability to model sea ice dynamics with sufficient accuracy, the marginal ice zone (MIZ) is particularly challenging. Because of strong fragmentation of the ice into many small floes, and highly energetic environment due to the presence of waves, it is a very difficult, unstable and dangerous location for field work. The amount of observational data from the MIZ is therefore very limited, and many seemingly basic processes are only poorly understood. This is the case if sea ice interactions with waves are concerned, i.e., the defining processes of the MIZ. For example, the functional form describing the rate of change of wave height with distance from the ice edge is far from established. Whereas most observations and models suggest exponential attenuation of waves propagating into the MIZ (e.g., Dumont et al., 2011), recent observations by Kohout et al. (2014) provide a different picture. During a storm event in the Southern Ocean, they observed exponential decay of wave height with distance for small waves, but much slower, approximately linear decay for waves exceeding 3 m in height. This led to the ice break-up hundreds of kilometers from the open ocean. Kohout et al. (2014) showed also the existence of strong correlation between the trends in the sea ice extent and significant wave height at various sections of the Southern Ocean during both ice growth and melting seasons. This illustrates the need for better understanding sea ice-waves interactions in order to improve the performance of climate models. The works by Dumont et al. (2011) and Williams et al. (2013) are a step in that direction, as they propose a floe-breaking parametrization for the MIZ based on the elastic-plate theory. Although quantitative observations are rare, many qualitative observations indicate that this theory correctly predicts one dominating floe size, related to the dominating wavelength, at least in situations with regular, unidirectional swell waves propagating into homogeneous ice. Indeed, striped floe patterns are observed repeatedly (see for example Fig. 3). In general, sea ice freshly broken by waves tends to be composed of polygonal floes with similar sizes (left image in Fig. 4). Much less is known about processes that produce wide, heavy-tailed floe-size distributions and rounded floe shapes typically observed in the MIZ, especially in its inner zone further from the ice edge (right image in Fig. 4).

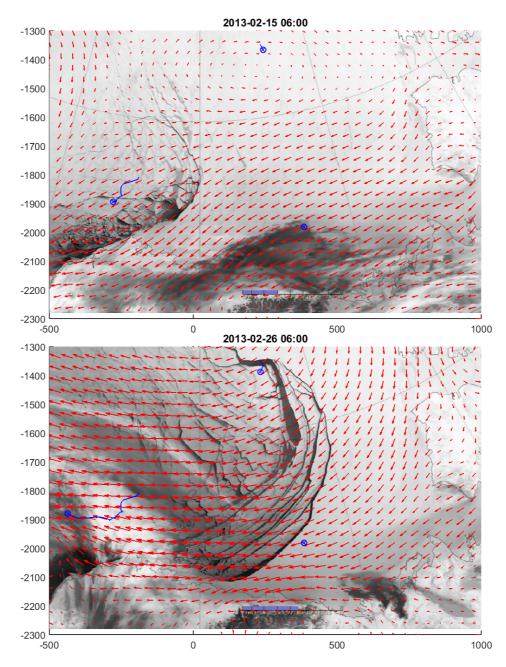


Figure 2: Beaufort Sea in Feb. 2013. Visible satellite images showing major sea ice break-up and deformation zones on 15 Feb (above) and 26 Feb (below). Arrows show the wind velocity from the NCEP-DOE reanalysis (Kanamitsu et al., 2002), blue lines and symbols – tracks and positions of IABP buoys. The x and y axes are in kilometers.

A working hypothesis in this project is that shearing of initially polygonal floes leads to the observed shape and size changes. The most probable source of this shear are across-ice-edge differences of the along-ice-edge ice velocity, especially when they are accompanied by overall convergence created by winds and/or currents. Similar mechanisms have been proposed recently by Åström et al. (2014) to explain the evolution of the distribution of fragment sizes created during calving of glaciers. Generally, processes shaping the size distribution of sea ice floes have become the subject of extensive observational and theoretical research (and workshops devoted specifically to this problem, e.g., at the Scottish Institute of Marine Science in Oban in July 2015), as more and more processes influenced by the floe-size distribution are becoming identified.

Among them is the atmosphere–ocean heat and momentum exchange, and the related mixing processes in the atmospheric and oceanic boundary layer. In a yet unpublished numerical work presented at the



Figure 3: Sea ice broken by swell. Photograph of sea ice floes forming parallel stripes – presumably a result of breaking due to regular swell waves with single dominating frequency. McMurdo Sound, Antarctica. (Source: http://www.norbertwu.com/nwp/conservation-environment-physical-ocean/glaciers&icebergs_web/detail.np/detail-36.html)

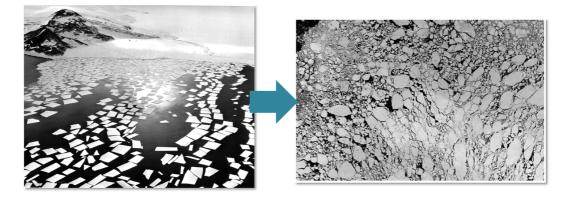


Figure 4: **Two different states of the marginal ice zone.** *Left*: polygonal floes broken by waves (Ross Island, 1961); *right*: rounded floes with a wide range of sizes after a long history of "grinding". (Sources: Antarctic Photo Library, U.S. Antarctic Program (left), Landsat (right)

last American Geophysical Union Assembly, Horvat and Tziperman (2014) demonstrated that large lateral gradients in surface heat flux and wind stress, associated with the "mosaic" pattern of sea ice and open water at medium ice concentrations, can either initiate or inhibit sub-mesoscale motion in the upper ocean, depending on the characteristic floe size. These sub-mesoscale motions may in turn modify the surface water temperature and thus the heat exchange with the atmosphere, closing the feedback loop. At present, larger-scale effects of these processes are poorly understood and are not taken into account in continuum models. Similarly, no parametrizations of analogous feedbacks in the lower atmosphere are available.

In terms of mesoscale atmospheric modeling in polar regions, the Polar Weather Research and Forecasting (Polar WRF) model (Bromwich et al., 2009; Hines et al., 2015) has brought several important achievements. It is a version of the "standard" WRF model with additional algorithms dedicated to the improved treatment of sea ice, land ice and snow, as well as the lower atmosphere in polar regions. Polar WRF has been used, e.g., to produce a high resolution reanalysis product for the polar and subpolar regions of the Northern Hemisphere – the Arctic System Reanalysis (Wilson et al., 2011, ; http://polarmet.osu.edu/ASR/).

However, none of the above-mentioned floe-size distribution related processes are included in this model. The list of similar processes and phenomena, taking place at medium ice concentrations and/or close to the ice edge, is long and includes, e.g., formation of narrow bands of ice floes. Whereas clustering of floes on the sea surface is itself a very basic process related to energy losses during collisions combined with size-dependent response of floes to wind and current forcing – as demonstrated by Herman (2011, 2012) – there seem to be a number of other mechanisms that may produce similar effects. For example, Wadhams (1983) developed a simple model explaining formation of ice bands by wind-generated waves during winds blowing from the ice towards the open water. Fujisaki and Oey (2011) used a much more complicated, coupled ocean–ice model to demonstrate ice band formation in convergence zones associated with lee waves during winds parallel to the ice edge. Apart from being interesting, these atmosphere–sea ice–ocean interactions have practical significance, because they directly and indirectly influence changes of the position of the ice edge due to dynamic and thermodynamic processes.

To summurize: The picture emerging from the ever growing amounts of more and more detailed data has led to a realization among scientists that in most cases sea ice cannot be treated as a viscous-plastic continuum covering the sea surface, because many large-scale properties of the ice cover result from its specific, "granular" nature and interactions at the floe–floe level. In short, the macro-scale, climate-relevant properties of sea ice are emergent properties, produced by smaller-scale and often poorly-understood processes. Deformation and fracturing of individual ice floes, and the related internal stress, influence the mechanical strength of the ice cover at the basin scale, as well as many other physical and geochemical processes taking place at the oceanatmosphere interface in polar and sub-polar regions. Moreover, these processes are interrelated, mutually connected by a number of feedbacks. Including them in climate models is a prerequisite for improving short-term and long-term predictions.

2.2 Pioneering nature of the project and impact of its results

Achieving the objectives of the proposed project is possible only by combining substantial progress that have taken place in two distinct disciplines – granular matter research and sea ice research. In both cases, these developments are related to both purely theoretical as well as practical aspects resulting from the technological development that enables more and more detailed observations and more and more effective numerical modeling of the analyzed phenomena. Especially in sea ice physics, recent achievements – described in the previous section – have been closely coupled to the increase of spatial and temporal resolution of both satellite data and numerical models.

Some of the most recent achievements of the physics of granular materials – important from the point of view of this project – are related to: relationships between the macroscopic properties of a given material, including its response to strain, with its properties at a "micro"-scale (i.e., physical properties of the material building the grains); the influence of polydispersity (variability of the grain size) on the properties of these materials; mechanisms of jamming in materials subject to compression and/or shear deformation; mechanisms of force and stress transmission in those materials and topological properties of the contact and force networks.

The pioneering nature of the proposed project lies in the combination of the cutting-edge results of both disciplines. This provides an opportunity to gain new insights into sea ice dynamics and related processes, but also to contribute to more general research on granular materials. The very strong polydispersity of sea ice, with floe sizes spanning a few orders of magnitude, makes it an extreme – and a very interesting – test case for granular-matter models.

The Principal Investigator has taken an active part in recent discussions among the sea ice community during conferences, workshops and other events. One of the most important was the "Mathematics of Sea Ice" conference in Vancouver in September 2015 (https://www.pims.math.ca/scientific-event/ 150924-cmsi), where she has given a plenary lecture. A notable continuation will be the series of events planned by the Isaac Newton Institute in Cambridge for the Autumn 2017 (https://www.newton.ac.uk/ event/sip). Four workshops are planned on "Multi-scale Modelling of Ice Characteristics and Behaviour", "Ice-Fluid Interaction", "Ice-Structure Interaction" and "Ice Fracture and Cracks" (the Principal Investigator is co-organizing one of them). Care will be taken that the activities within the proposed project remain within the scope of the most actively pursued sea ice research directions, and that the results are discussed with the most active researchers in the field.

On the other hand, in the last years the Principal Investigator has been actively trying to carry the fascinating problems of sea ice dynamics to researchers working on granular materials, discrete-element methods and statistical physics, by publishing in interdisciplinary journals and attending large interdisciplinary conferences (recently: the 13th US National Congress on Computational Mechanics in San Diego in July 2015 and the 4th Conference on Particle-Based Methods in Barcelona in September 2015; both invited talks). The goal has been both to popularize sea ice research and to keep up-to-date with the latest achievements of the relevant disciplines. As already mentioned, this strategy is a prerequisite to the successful completion of the project objectives and therefore it will be continued during the realization of this project.

The project concentrates on processes for which no consistent, practically applicable models exist at present. Thus, it is a basic research, and its main purpose, apart from understanding these processes, is to provide foundations for algorithms that can be practically applied in large-scale sea ice and climate models in the future.

Implementation of new features in the DESIgn sea ice model will not only facilitate the completion of tasks within this project, but will bring certain, very positive "side effects" by making the model applicable to a wider range of problems, like for example an analysis of iceberg motion in sea ice, which requires at least a simple model of the upper ocean in order to specify the integrated forcing acting on an iceberg underwater (recently, the PI was approached by glaciologists who expressed interest in applying DESIgn for this purpose).

Similarly to the present version, the new code of the model will be made freely available to the sea ice community.

The results will be presented at a number of international conferences and published in high-impact scientific journals.

3 Work plan

3.1 State of preliminary and initial research

As already mentioned in the first part of this proposal, a discrete-element model will be the main tool used to accomplish the goals of the project. Discrete-element modeling of sea ice has been the main area of research of the Principal Investigator within the last couple of years. As part of this work, increasingly more advanced numerical sea ice model has been developed, starting from a simple event-driven algorithm suitable for simulating low-concentration sea ice as a granular gas (Herman, 2011, 2012), up to the latest version applicable to a wide range of sea ice types and forcing conditions (Herman, 2013b,a,c). The most recent code, called DESIgn (Discrete-Element bonded-particle Sea Ice model), is freely available as a toolbox for the LIGGHTS numerical library and can be accessed at http://herman.ocean.ug.edu.pl/LIGGGHTSseaice. html. A full description of the model, together with a technical documentation and example input files, has been published as a discussion paper in Geoscientific Model Development Discussions (Herman, 2015); at the time of submission of this proposal, the final version of this paper undergoes final stages of the review process for a regular issue of GMD.

The present version of DESIgn enables two-dimensional (2D) computation of sea ice deformation and damage. Preliminary simulations performed for the 2013 Beaufort Sea ice fracture (Figs. 5 and 6) show that even the present model version can be applied not only to idealized configurations – like those described in the above-cited papers – but also to realistic, larger-scale settings. However, this applicability is limited to short time periods due to the lack of a number of important processes, especially pressure ridging, which is not implemented at present. This leads to undesired model behavior, e.g., to progressive accumulation of unrealistically high stress in compressed grains. Thus, further developments are required to broaden the range of the model applications.

Although in principle DESIgn is two-dimensional, its latest version enables calculation of bending and twisting moments acting on the ice subject to ocean surface waves (Herman, 2015). These moments, related to the curvature of the sea surface, are calculated in a rather simplistic way. Moreover, a number of other significant sea ice–waves interaction mechanisms are not taken into account, and the whole wave-related part of the model should be regarded as experimental. However, it is a good starting point for further developments, especially from the technical, computational point of view: all basic variables storing the horizontal components of the moments, tilt of the grains, sea surface elevation, and so on, are already defined and properly integrated into the code. What remains to be done is thus a conceptual, but not a computational challenge.

Finally, a large group of tasks within the proposed project involves numerical modeling of the atmosphere (Section 3.2.5). As mentioned earlier, the Polar WRF model will be used for that purpose. The Principal Investigator has experience with this model from the EU project SatBałtyk, in which she was responsible for configuring, calibrating, validating and running the model for the Baltic Sea area. The model runs operationally at the Department of Physical Oceanography, IOUG, and its results from the period 2010–present are available through the SatBałtyk Internet platform (http://satbaltic.iopan.gda.pl). Additionally, the PI used WRF to analyze the influence of sea ice on the lower troposphere and on the atmosphere–sea ice–ocean interactions in the northern Baltic Sea.

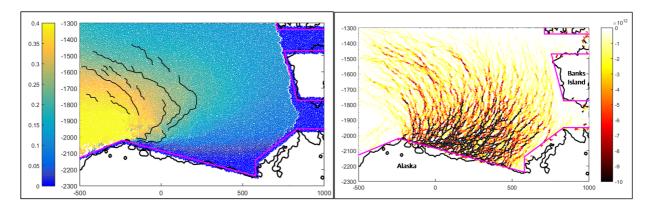


Figure 5: Test results of DESIgn Beaufort Sea simulations. *Left*: modeled sea ice velocity (in m/s), with major bond-breaking zones highlighted in black; *right*: bond-transmitted compressive stress acting on the grains. Magenta lines show the position of coastlines used in the model.

3.2 Outline of the work plan

The planned tasks within the project have been divided into 5 thematic groups:

3.2.1 Sea ice in the marginal ice zone

This group of tasks includes the development of theoretical foundations and numerical implementation of algorithms related to sea ice interactions with waves, as well as the analysis of other processes leading to the breaking of floes and thus shaping the floe-size distribution in MIZ. The specific tasks are:

- 1. Formulating equations describing the vertical motion of grains on the sea surface and implementing them in the code.
- 2. Detailed analysis of spatiotemporal variability of wave-induced velocities and stresses acting on grains and bonds in (horizontally) 1D and 2D configurations.
- 3. Implementation of additional aspects of sea ice–waves interactions, including modification of the wave parameters resulting from the presence of sea ice.
- 4. Formulation of relationships between the wave forcing and the resulting floe-size distribution with the purpose to propose parameterizations suitable for continuum sea ice models.
- 5. Numerical analysis of floes' "grinding" and diminution by shear in the inner marginal ice zone.

3.2.2 Ridging parametrization and thermodynamics

This group of tasks is related to two different groups of physical processes – formation of pressure ridges due to sea ice deformation, and changes of the sea ice volume due to freezing/melting. They are treated together because at the technical level their implementation requires similar changes to the model code. Specifically, the tasks in this group include:

- 1. Implementation of new functionalities required by both the ridging and the thermodynamic schemes, including but not limited to time-dependent grain and bond thicknesses, grain radii and bond widths, as well as improved handling of new bond formation during a simulation.
- 2. Testing of various approaches to ridging parametrization algorithms suitable for DESIgn, from simple ones, in which the material of bonds breaking in compression is used to increase the thickness of the grains involved, to more complex ones, in which additional grain properties are modified depending on the nature of stress acting on them.
- 3. Analysis of the influence of the ridging parametrization on sea ice behavior in a number of simple configurations.

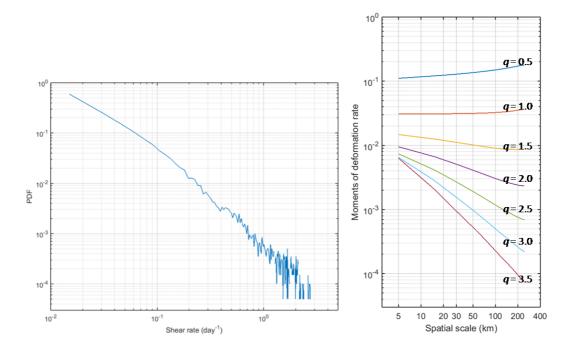


Figure 6: Statistical properties of sea ice deformation simulated with DESIgn. Left: pdf of the modeled shear rate (in day⁻¹); right: moments of deformation rate in function of the spatial scale (see Herman and Glowacki, 2012, for analogous moments based on satellite data).

4. Formulating and implementing functions describing temporal changes of the grain and bond properties due to the prescribed air/water temperature and/or atmospheric/oceanic heat fluxes.

3.2.3 Beaufort Sea case study

This group of tasks concentrates on the application of the DESIgn model to the analysis of the sea ice break up event in the Beaufort Sea in winter 2013. These tasks are dependent on previous *completion* of tasks from section 3.2.2 above. They include:

- 1. Configuration and calibration of the model parameters (based on the already prepared and tested preliminary configuration, Fig. 5) and preparation of additional input, calibration and validation data from available sources.
- 2. Detailed analysis of sea ice velocity, stress, bond breaking patterns and deformation rates during consecutive stages of the break-up event.
- 3. Additional simulations with modified selected model parameters in order to test hypotheses related to the causes of the exceptional sea ice break-up in winter 2013.

3.2.4 Numerical aspects of the DESIgn model

This group of tasks includes development, implementation, testing and dissemination of the next version(s) of DESIgn, as well as developing efficient visualization tools for DESIgn results. Specifically, the tasks are:

- 1. Implementing and testing of new model features, optimizing their computational efficiency, identifying and removing bugs, etc.
- 2. Updating the code of DESIgn to new versions of the LIGGGHTS library, testing if the new DESIgn features are compatible with new features of LIGGGHTS.
- 3. Preparing the updated technical documentation of the model, as well as updating its home page.
- 4. Improving the existing and designing new tools for visualizing the results of the simulations in the form of images and animations.

3.2.5 Sea ice-atmosphere interactions

Tasks in this group are related to modeling of sea ice interactions with the ocean and the atmosphere. They include:

- 1. Small-scale WRF simulations of the atmospheric boundary layer over inhomogeneous sea ice with prescribed ice concentration and floe-size distribution.
- 2. Developing and implementing framework for coupled WRF–DESIgn simulations and for including simplified ocean mixed layer model (based on the existing 1D model of WRF).
- 3. Coupled WRF–DESIgn–ocean mixed layer simulations in situations with medium ice concentration.
- 4. Analysis of atmosphere–sea ice–ocean interactions close to the ice edge and their role in shifts of the position of the ice edge and in formation of ice bands.

4 Research Methodology

4.1 Methods used in the five main groups of project tasks

As already mentioned in previous sections, the main tool used in this project will be a discrete-element bonded-particle model of sea ice. The present version of the model, called DESIgn, is described in detail in Herman (2015) and in the technical documentation available at http://herman.ocean.ug.edu.pl/ LIGGGHTSseaice.html. The code of the model is based on the LIGGGHTS library (LAMMPS Improved for General Granular and Granular Heat Transfer Simulations;

http://www.cfdem.com/liggghtsr-open-source-discrete-element-method-particle-simulation-code), which in turn is based on LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator; http: //lammps.sandia.gov/). All functionalities of the sea ice toolbox are defined as derived from classes already used in LIGGGHTS. Thanks to the modular structure of LAMMPS and LIGGGHTS, extending the model with new features is relatively straightforward. The work within this project will require modifications to certain existing features (for example, allowing for time variability of the properties of grains and bonds in order to take into account ridging, freezing, etc.; or proper handling of the vertical component of the grains' motion on waves, which is treated rather simplistically in the present version), as well as implementation of entirely new features (for example, a simple model of the ocean mixed layer, allowing for calculation of the current speed – in the present version it has to be specified *a priori*). The implementation of the new features will be done mainly within the second and fourth group of tasks (see previous section). Importantly, within the fourth group, updates to the recent versions of the LIGGGHTS library will be made, so that DESIgn remains compatible with that library. As new versions of LIGGGHTS are published at least once a year, these tasks will be performed a few times within the time period of this project.

Within the first group of tasks, related to the marginal ice zone and sea ice–waves interactions, simulations with DESIgn will be aided by simplified 2DV simulations in Matlab, in which an individual sine wave, or a group of sine waves, propagates through a chain of bonded grains arranged along a straight line. By varying the properties of the wave(s) and of the grains/bonds, the response of the modeled ice will be analyzed from the point of view of the space-time variability of stress, which decides upon breaking patterns and thus the floe-size distribution. In this simplified version, the problem can be formulated as a set of ordinary differential equations that are easier to analyze numerically and semi-analytically than the full computations, which will be performed at further stages. The results will be compared with those of the elastic-plate theory and other models used in the literature to estimate the floe-size distribution from given wave and ice properties (see, e.g., Williams et al., 2013).

In the present version of DESIgn, the waves' parameters (period, amplitude, etc.) have to be prescribed within the whole model domain. Moreover, a simple deep-water dispersion relation is used. This is unrealistic, and will be replaced by a model in which the presence of ice will be taken into account by calculating the waves' parameters.

Further, within task group 1, simulations of "grinding" of the ice floes (initially broken by waves) will be performed in order to analyze processes that lead to the formation of the heavy-tailed floe-size distributions observed in the marginal ice zone. To this end, relatively simple simulations are planned, in which a set of rectangular floes, similar to those seen in the left panel of Fig. 4, are subject to shear deformation, which leads to "grinding" and diminution of the floes. The model setup used in initial tests is shown in Fig. 7.

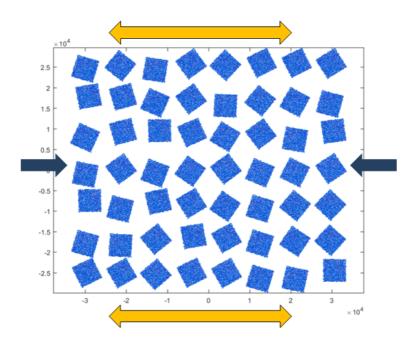


Figure 7: Model setup for "grinding" simulations. A set of rectangular floes, each composed of many connected grains and subject to deformation shown with arrows.

Each floe is defined as an assemblage of bonded grains, and a narrow, uniform grain-size distribution is used in order not to influence the final result by specifying a wide size distribution already as input. The floes are sheared by periodically moving the upper and lower model boundaries in opposite directions (yellow arrows in Fig. 7). Additional forcing is specified along the left and right boundaries to prevent the floes from leaving the domain. After initial tests, this simple configuration will be extended in order to obtain realistic forcing acting on the ice in the inner parts of the marginal ice zone.

As far as the tasks in group 3 are concerned (Beaufort Sea simulations), observational data from a number of sources will be required as either model input, for validation purposes and/or to provide background information on the processes in the ocean-sea ice-atmosphere before and during the events of interest. The data used for this purpose will include: (i) bottom topography from ETOPO2v2 gridded data (http://www. ngdc.noaa.gov/mgg/global/etopo2.html); (ii) AVHRR satellite imagery of sea ice; (iii) trajectories of the buoys of the International Arctic Buoy Program (http://iabp.apl.washington.edu/); (iv) air temperature, sea-level pressure and surface wind speeds from the NCEP-DOE reanalysis data (Kanamitsu et al., 2002); (v) tidal current velocities from the polar tidal models of the Earth and Space Research Institute (https://www. esr.org/ptm_index.html); (vi) sea ice thickness estimations from available satellite data and numerical models; (vii) sea ice velocity at the open boundaries of the model area from available numerical models; (viii) sea ice concentration and distribution of first-year and multi-year ice from the OSI-SAF data (http: //www.osi-saf.org/; http://osisaf.met.no/p/ice/). All these data types are already at the disposal of the PI; most have been already preprocessed, e.g., spatial interpolation onto the model grid has been done.

The model domain will cover the region shown in Figs. 2 and 5, i.e., 1500×1000 km. Fig. 5 shows also the position of the coastlines used in the model. All grains located landward from these lines are considered as land-fast ice and their positions are not updated during the simulation. Due to the very large size of the domain – much larger than used in hitherto applications of the model – the grains in this case will be large, not smaller than a few hundreds of meters. The model will be calibrated to produce realistic sea ice velocities and deformation patterns (as observed in satellite imagery). A series of simulations with different parameters, initial conditions and/or forcing will be used to analyze the influence of these factors on the details of the fracture event.

The tasks in group 5 are the only ones that require modeling not only with DESIgn, but also with an atmospheric model. For this purpose, Polar WRF (Weather Research and Forecasting; Bromwich et al., 2009; Hines et al., 2015, see also http://polarmet.osu.edu/PWRF/) will be used, i.e., the version of the WRF model dedicated to the polar regions due to, first, improved treatment of sea ice, and second, parameterizations suitable for specific features of the, usually very stable, atmospheric boundary layer over snow- and ice-covered

regions. Within this project, very-high-resolution simulations of the lower atmosphere will be performed in order to identify and analyze sub-mesoscale processes associated with nonuniform distribution of sea ice on the sea surface. After an initial calibration to available observational data (nested simulations of a small area within a larger domain), a series of simulations will be performed for a number of observed and artificially generated sea ice "maps", showing the positions of individual ice floes on the sea surface. Variability of surface wind speed, heat and moisture fluxes, vertical stability, etc., will be analyzed in order to formulate simplified relationships between the sea ice concentration and floe-size distribution on the one hand, and the area-averaged values of the atmospheric variables on the other hand.

Further, coupled DESIgn–WRF simulations are considered, in which the surface wind will be passed from WRF to DESIgn, and the positions of the sea ice floes will be passed from DESIgn to WRF. This technique will be used, among other things, to analyze the process of formation of bands of ice floes on the sea surface at the edge of the marginal ice zone, and other aspects of atmosphere–ice–ocean interactions close to the ice edge.

4.2 Computational equipment and software

Both DESIgn and WRF are extremely computationally expensive. Therefore, sufficient computational power is the major prerequisite for successful completion of the project objectives. Fortunately, thanks to a number of large projects that have been conducted at the Department of Physical Oceanography IOUG in recent years, we have enough computational power at our disposal: 25 Intel Xeon class servers with 8+8+12+12+64+80 = 184 physical cores with 12+12+24+24+128+20*8 = 360 GB operational memory and over 100 TB of disk space. The servers use Ethernet 1GB and infiniBand 20GB DDR and 2 Tesla 2075 cards. Additionally, the Principal Investigator has experience in compiling and running the sea ice model at the machines of the Academic Computer Center in Gdańsk (TASK, http://task.gda.pl/) – part of the simulations described in her previous publications have been performed there. In recent months, a new computational server, called TRYTON, has become available at TASK, which is the first computer in Poland with more than 1 PFLOPS computational power (~ $1.2 \cdot 10^{15}$ operations per second).

Therefore, sufficient computational resources shouldn't be a problem for the project realization. We only plan to purchase two workstations for the two new members of the team, i.e., the PhD student and the MSc student (Co-Investigators no. 2 and 4) in order to provide workplace for them. The work stations should be powerful enough to perform pre- and postprocessing of data, data analysis and visualization, and test model runs. Detailed specification is provided in the list of equipment to be purchased.

We have a licence for the Intel Compiler on our servers, necessary for compilation of both DESIgn and WRF. The Principal Investigator uses Matlab for her work for many years and in that time she has built a large library of scripts and functions for data processing, analysis and visualization. It is desirable that other participants of the project have access to these tools and that they can extend and modify them. Thus, the purchase of 2 individual licences of Matlab is planned, each with a set of basic toolboxes (e.g., Statistics Toolbox, Optimization Toolbox, Signal Processing Toolbox). Additional open-source programs will be used for the purpose of the visualization and dissemination of the modeling results in the form of figures and animations.

4.3 Division of the work among the project participants

Until now, the development of the DESIgn model has been the work of a single person (the proposed Principal Investigator). Wide interest in the model within the sea ice modeling community indicates the need for further development of this model. However, this is possible only if additional persons get involved in the work. As can be seen from section 4.2 above, the resource limiting further development in our case is not the computational equipment, but human resources. This is the reason why personal costs are the main component of the overall costs of this project. The PI believes that investing in young researchers is the most valuable kind of investment in her work. It is planned to engage: (i) one PhD student with background in physical oceanography and/or atmospheric science, with at least basic programming and numerical-modeling skills, preferably with some experience in atmospheric modeling – for the whole period of 3 years; (ii) one MSc student with background in physical oceanography, physics or computer science, with at least basic programming skills – for the period of 2 years, corresponding to the duration of Master-level education in Poland. Additionally, a very important member of the team, involved mainly in the computational and numerical aspects of the project tasks, will be Jakub Zdroik (MSc), the person who has been responsible for the maintenance of the computer resources at the Department of Physical Oceanography, as well as for all our

operational algorithms of satellite- and model-data acquisition, processing and visualization. In particular, he has been the author of the whole operational system developed and run at the University of Gdańsk as part of the recent SatBałtyk project.

The tasks of the individual project participants are:

- 1. Principal Investigator:
 - coordinating the project,
 - supervising of the PhD dissertation of Co-investigator no. 2 and co-supervising of the work of Co-investigator no. 4,
 - leading and participating in the theoretical and numerical work in all project tasks,
 - performing the majority of theoretical and numerical work within tasks 1 and 2,
 - preparing of publications and conference presentations, presenting the results at international conferences and workshops.
- 2. Co-Investigator no.2 (PhD student):
 - participating in the theoretical and numerical work in all project tasks,
 - performing the majority of theoretical and numerical work within task 5, which will be the main subject of his/her doctor thesis (completed presumably after the project finishes),
 - preparing of publications and conference presentations, presenting the results at international conferences and workshops.
- 3. Co-Investigator no.3:
 - co-supervising of the work of Co-investigator no. 4,
 - participating in numerical work in all project tasks,
 - performing the majority of work within task 4,
 - developing tools for efficient and informative visualization of the modeling results, especially the output of DESIgn simulations, for the purpose of publications, conference presentations, and dissemination on the Internet.
- 4. Co-Investigator no.4 (MSc student):
 - participating in the theoretical and numerical work in tasks 3 and 4,
 - preparing MSc thesis based on his/her work on task 3,
 - participating in preparation of publications and conference presentations.

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