Vacuum chamber conditioning and saturation simulation tool (VacuumCOST): Enabling time-dependent simulations of pressure and NEG sticking in UHV chambers

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ABSTRACT

Modern particle accelerators, synchrotrons, and other machines requiring UHV frequently make use of NEG coatings to achieve low pressures and resulting high beam stability and lifetime. It is the nature of NEG pumps and coatings, that a limited amount of gas can be pumped before saturation is reached, at which point the NEG must be re-activated to pump efficiently again. While the pumping mechanism and absorption limits are well understood and software packages exist for simulating the steady-state vacuum systems, there is a need for simulating the temporal evolution of the pumping capability of NEG coatings in regions of high outgassing rates such as near crotch absorbers. This paper presents a simple framework, written in Python, for running time-dependent simulations of NEG-coated vacuum systems in molecular flow, by making use of the command-line interface of the already widely used MolFlow simulation software. It also compares simulation results with accelerator pressure measurements.

1. Introduction

Getters are materials that are able to adsorb gas molecules, thereby acting as a pump by binding the molecules in the system and removing them from the gas dynamics of the vacuum environment [1]. To facilitate the chemisorption process, their surfaces must be chemically reactive, limiting their pumping capacity to approximately a monolayer, the exception being H_2 which dissociates on the surface before the H atoms diffuse into the bulk. In contrast to evaporable getters that deposit a new layer of getter material to enable further pumping, Non-Evaporable Getter (NEG) materials can diffuse the adsorbed layer into their bulk when heated to their activation temperature, freeing pumping sites to be used again [2]. NEG coatings are now commonly used for producing high-quality vacuum in large systems such as synchrotron light sources and particle accelerators [3].

As a consequence of the formation of an adsorbed surface layer, the pumping speed of a NEG surface is reduced as gas is pumped, and eventually the molecule sticking probability s reaches zero when all active pumping sites are occupied by sorbed molecules. At the same time, for the case of accelerators where photo-stimulated desorption (PSD) plays a role, the PSD yield decreases over time as the areas illuminated by synchrotron radiation (SR) are conditioned [4].

To understand how a vacuum system evolves over time, it is thus necessary to perform simulations, taking into account both how the introduction of molecules to the system (through injection of gas, PSD, or other mechanisms) varies over time, as well as how the pumping efficiency of the different areas in the system are affected by current and previous conditions. The Vacuum chamber conditioning and saturation simulation tool (VacuumCOST) is designed to enable these simulations through the use of a time-marching method. A similar technique has recently been developed elsewhere [5] but VacuumCOST makes this functionality available open source.

2. Description of simulation code

The backbone of the simulations are the tools MolFlow and Syn-Rad. Both of these programs are well-known, commonly used, and have been described extensively elsewhere [6–9]. They are designed for simulating steady-state and rapid time-dependent systems, but the latest version of MolFlow includes a command-line interface (CLI) so repeated simulations can be performed with different surface and gas properties, updated automatically through a script in Python.

2.1. Simulation procedure

VacuumCOST comprises a collection of Python scripts to configure simulation settings, perform the actual simulation at the required temporal resolution, and to process and plot the results. In each iteration of

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the simulation, the desorption rate and sticking probability of all facets in the model are updated based on the time step under consideration and the results of the previous simulation iteration.

2.1.1. NEG saturation models

While the user can easily add additional models for the sticking coefficient, or modify the existing models, the standard simulation procedure consists of simulations of CO and H_2 with a simple model assuming a linear decrease of CO sticking coefficient as function of surface coverage while H_2, following a second order kinetic equation for dissociative chemisorption [10], depends on the CO coverage squared. The sticking probabilities are thus

$$s_{CO} = s_{CO,0} \left(1 - \frac{Q_{CO}}{Q_{CO,ml}} \right) \tag{1}$$

$$s_{H_2} = s_{H_2,0} \left(1 - \frac{Q_{CO}}{Q_{CO,ml}} \right)^2 \tag{2}$$

where Q_{CO} is the amount of pumped CO molecules. As standard values $Q_{CO,ml} = 2 \times 10^{15}$ molecules/cm^2 is used as the density of adsorbed molecules corresponding to one monolayer, while the initial sticking probabilities are $s_{CO,0} = 0.7$ and $s_{H_2,0} = 8 \times 10^{-3}$ [3]. Although dissociated hydrogen atoms diffuse into the bulk of the NEG, H_2 sorption requires active surface sites, hence the dependency on CO surface coverage for the sticking probability of H_2. For this reason, a simulation of the geometry for CO must be performed before H_2 can be simulated.

2.1.2. Calculating PSD

For the case where outgassing rate is determined by photo-stimulated desorption, a data file for the desorption yield is required. Between each set of data points, power law functions are fitted to allow for interpolation of the outgassing rate for any SR dose density, or extrapolation in case the dose density simulated does not fall within the supplied data range. When simulating a geometry in SynRad each facet is divided into a number of texture cells. The user must export data on the texture cell area and SR flux which will be loaded by VacuumCOST and stored internally for use in the simulation. For each iteration of the simulation, VacuumCOST will calculate the SR dose density based on these values and the time step considered. From the fits to the desorption yield, the outgassing rate for each texture cell of each facet is determined.

2.1.3. Iterating procedure

The user can supply pre-determined time steps to consider for the simulation if so desired, but the primary use case is utilizing the built-in feature to automatize the simulation, and let VacuumCOST determine the temporal resolution required to satisfy criteria on the maximum allowable change in sticking coefficient and outgassing rate between two subsequent iterations. In this case the total simulation time is specified, along with aforementioned criteria. The initial state of the system may be defined such that the facets in the geometry have varying levels of conditioning prior to the launch of the simulation. In each iteration, the new sticking coefficient of each facet and the new outgassing rate from each texture cell, is calculated depending on the time passed between two iterations and the number and location of pumped molecules. If any criterion is not met, an intermediate time step is injected halfway between the previous and current time steps and the calculation is performed again. In this way, the temporal resolution at each time slice of the simulation is automatically determined to satisfy the user-specified requirements. The required temporal resolution is not constant throughout a simulation but rather much higher initially. Once CO has been simulated, a simulation for H_2 can be performed but in this case the time steps determined for CO are used and no additional time steps are injected regardless of the relative change in sticking coefficient and outgassing rate.

2.2. Limitations

Unlike PSD, which is defined for individual cells on a facet, the sticking coefficient of a facet currently applies to its entire surface area. In order to ensure a sufficient spatial resolution, large facets should be avoided, which means that large or complex geometries may need to consist of hundreds of thousands of facets, resulting in large file sizes and long simulation times. This is, however, planned for implementation in a future version of MolFlow with integrated iterative simulations. In addition, the criteria for maximum change in sticking coefficient and outgassing rate must be sufficiently relaxed that the required temporal resolution is no higher than 1 iteration/s. In practice thresholds of 1% change in sticking coefficient and 5% change in outgassing rate between iterations can safely be used. Naturally, the results are also highly dependent on whether the sticking model being used is an accurate representation of the sticking probability of the surface.

3. Simulation results

During code development, VacuumCOST has been tested on a number of different geometries to probe weaknesses and improve usability. As a demonstrator of the tool, a simulation of the region around a crotch absorber in the MAX IV synchrotron facility will be used.

3.1. Demonstration case: MAX IV crotch absorber

This system is used as a test case since it is already in operation and pressure measurements are available to compare with the pressure evolution predicted from simulations. An illustration of the region near the crotch absorber is shown in Fig. 1.
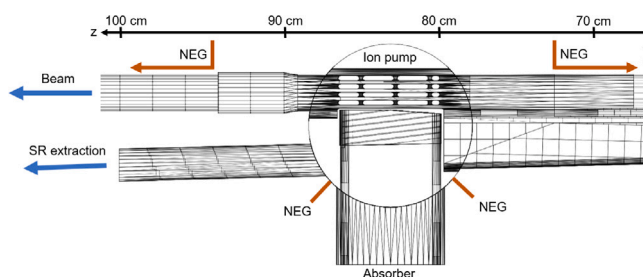

Fig. 1. Top view of a section of the geometry simulated. The beam direction and NEG-coated areas are indicated. The circular shape in the center is the outline of a NEG-coated vacuum chamber also fitted with an ion pump.
Source: Figure adapted from [9].

For the simulations, the standard beam current of 250 mA is used [11]. The model is located largely along the z-axis of the MolFlow coordinate system, with the ion pump at $z = 83.5$ cm. The minimum spatial resolution in the z-wise direction is 0.5 cm^{-1} (maximum facet length of 2 cm) but it is higher in some areas upstream of the absorber due to the non-parallel details of the geometry.

For desorption yield estimation, data for OFHC Cu is used [12]. Fig. 2 shows an example of how the VacuumCOST fits to the data. Within the available data range interpolation between points is used. For doses outside the range extrapolation to either side is used based on the slope of the curve most closely matching the dose in question.

The system was simulated using thresholds for the maximum change in sticking coefficient and desorption rate between iterations of 1% and 5%, respectively, resulting in a total of 781 time steps to simulate 12000 h corresponding to 3000 Ah at 250 mA. The evaluation of each time slice's adherence to the criteria and progression of the simulation
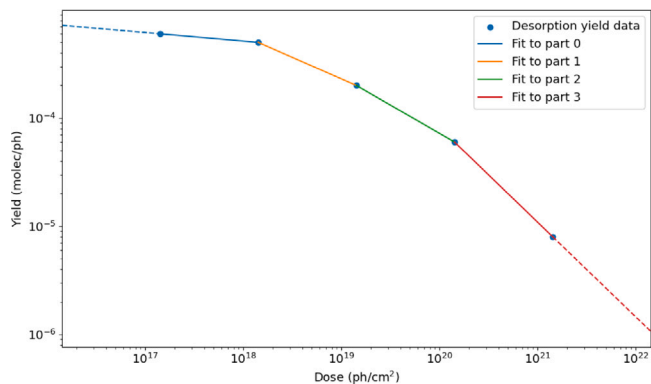
Fig. 2. Example of fits to each set of data points in desorption yield data used to determine the PSD yield for any dose. Extrapolation outside data range is indicated by dashed lines.

Fig. 4. Surface coverage along the length of the simulated system shown for 10 time slices.

Fig. 5. Fraction of absorbed molecules as function of position for 10 time slices.

as described in Section 2.1.3 is shown in Fig. 3. Initially time slices are reduced by half until the temporal resolution between steps 1 and 2 is sufficient to satisfy the criteria. After this, VacuumCOST iterated through testing 1561 time steps in total before settling on 781 steps for the actual simulation. The figure also shows the outgassing rate determined by the results of the SynRad simulation and the fits shown in Fig. 2 for each of the time slices of the simulation.
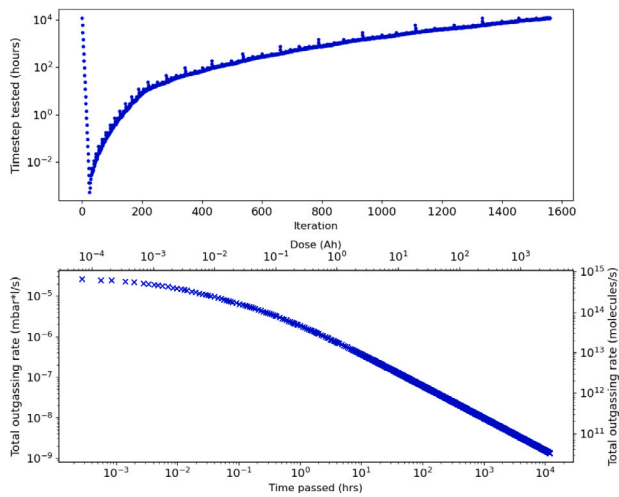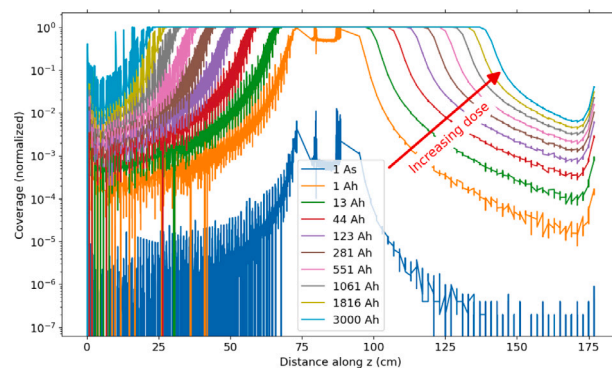

Fig. 3. Top: Illustration of the time steps tested and the temporal progression in each iteration of the simulation. Bottom: Evolution of the total outgassing rate in the simulated system as function of time and dose.
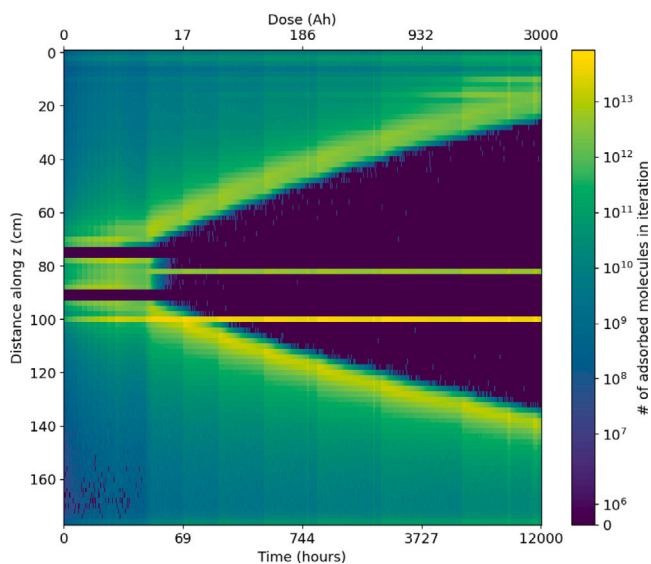

Fig. 6. Illustration of the number of absorbed molecules as function of time and position. The reduction in molecule absorption near the crotch absorber is clearly seen towards the right hand side of the figure.

The surface coverage along the length of the simulated system is shown in Fig. 4. A subset of 10 time slices are plotted. At the first time slice (after 2 s) only the facets near the crotch absorber have any coverage and it is less than 1%. As time progresses, those facets are saturated, and the surface coverage front increases outwards on either side of the absorber. Fig. 5 is similar to Fig. 4 but here the fraction of absorbed molecules is shown, indicating the point of maximum pumping for each time slice. Initially almost 100% of molecules are pumped near the absorber but the pumping location widens and migrates away from the absorber over time.

Fig. 6 shows a 2D plot of the number of pumped molecules in each time step as function of position in the geometry. A few horizontal bands of near constant pumping can be identified. One band represents the location of the ion pump with constant pumping speed. Another is a facet with constant sticking probability of 0.1 representing a connection to another part of the system in equilibrium with the simulated section. Although the outgassing rate in the system decreases over time, the

fraction of molecules pumped at these locations approaches unity as time goes to infinity, which is why the absolute number of pumped molecules remains more or less constant throughout. The bands with no pumped molecules are a non-NEG coated non-pumping parts of the system. The rest of the system is NEG coated and a clear reduction in the number of pumped molecules near the absorber can be seen, after the facets in the vicinity are saturated. This area is surrounded by a front of an increased number of pumped molecules, expanding as the saturation front moves.

Similar to Fig. 6, Fig. 7 shows the evolution of sticking coefficient as function of location and time. Non-NEG coated areas are not shown, hence the horizontal white bands in the figure. The saturation front is here very clear, giving rise to the reduced number of pumped molecules as seen in the previous figure. A contour line shows the point of 99% surface coverage.
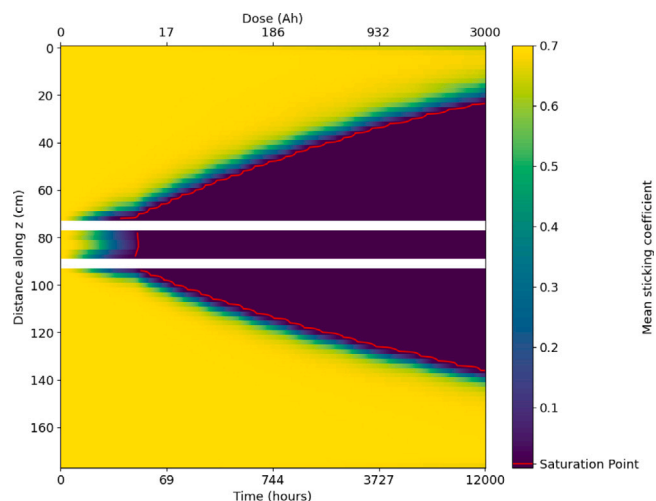

Fig. 7. Illustration of the sticking coefficient as function of time and position. The contour line showing saturation point corresponds to 99% surface coverage.

Fig. 8 shows the movement of the saturation point, starting near the crotch absorber and moving almost symmetrically upstream and downstream, along with the remaining sticking capability relative to the initial capability. On a linear scale plot, it is evident that the largest
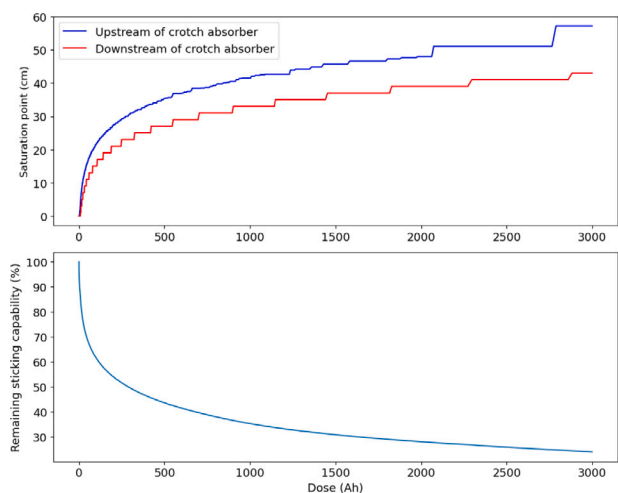

Fig. 8. Top: The progression of saturation (99% level) of the NEG-coating on either side of the crotch absorber. A part of the geometry upstream of the absorber has larger than 2 cm spatial resolution. Bottom: Remaining sticking capability in the simulated geometry.
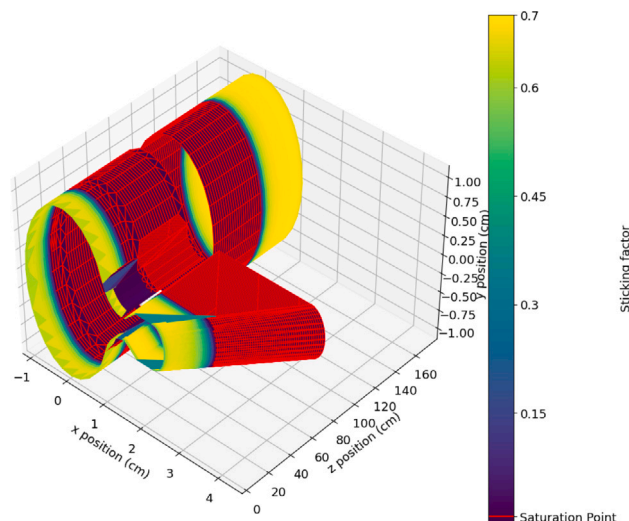

Fig. 9. 3D plot showing the sticking coefficient after 3000 Ah with the central part of the geometry removed for increased visibility of the NEG-coated surfaces. Facets with $\geq$99% saturation are marked with red edges. Note that the aspect ratio is far from 1. See Section "Code availability" for an animation from $t = 0$.

effect occurs initially when the PSD yield is high, whereas conditioning quickly reduces the gradient of reduction of sticking coefficient. The geometry is plotted in Fig. 9 with the colors indicating the final sticking coefficient after the simulation. The resulting partial pressures as function of dose are shown in Fig. 10. Also shown is the simulated normalized pressure rise as would be measured by a gauge in the storage ring above the crotch absorber, along with pressure rise data averages from the storage ring published in [11]. The simulated pressures are shown both for the sticking models outlined in Section 2.1.1 included in VacuumCOST with two different initial sticking probabilities for CO, and for sticking models based on fits to empirical data [3,13–15].
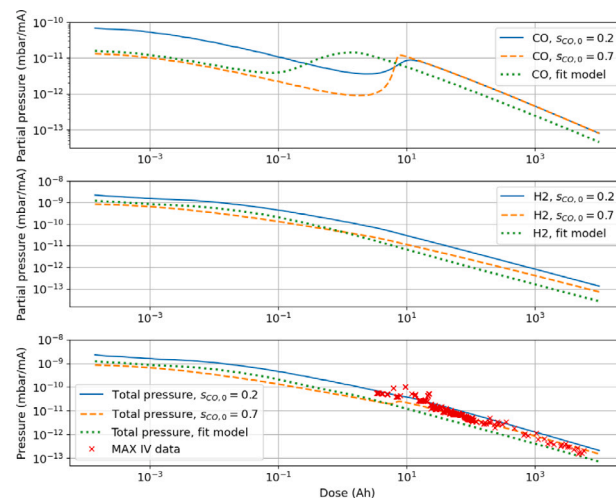

Fig. 10. Top and mid: Evolution of partial CO and H_2 pressures for different sticking models normalized to the beam current. Bottom: Simulated pressure rise as would be measured in the storage ring (nitrogen equivalent). Measured data from extractor gauges [11] is over-plotted for comparison.

The bump in the CO pressure appears as the first facets begin to saturate. This causes a localized pressure increase in the region that also houses the pressure gauge. While H_2 pumping speed is a function of the CO surface coverage, the generally low sticking coefficient of H_2 reduces its sensitivity to localized areas of saturated facets.

4. Computation time

The time required to run a VacuumCOST simulation is highly dependent on the geometry under consideration, the temporal resolution required, the total simulated time, the desired level of statistical variance, and the CPU speed of the computer used. The simulation described here consists of a geometry with 10,701 facets. On a relatively modern laptop computer (Intel Core i5-1135G7), the simulation took around 30 h for each of the gas species simulated.

5. Discussion

The defined spatial resolution and the acquired temporal resolution are sufficient to accurately simulate the conditions in the MAX IV storage ring in terms of predicting the gradient of the pressure evolution with accumulated dose. The results do, however, highlight the importance of using accurate sticking models and PSD yield data, as the simulated pressure is highly dependent on these parameters. Having correct parameters along with a valid geometry enables simulations that can accurately reflect the physical system in a reliable manner.

As the standard metric for determining whether to inject a time step, the mean change in sticking coefficient between the subset of facets that pumped molecules is used. The user may want to change this to the median change, maximum change for any one facet, or even a more advanced weighted metric, to ensure that no facets are instantly saturated due to the majority only pumping relatively few molecules, thereby reducing the mean change in sticking coefficient to below the threshold. The choice is a trade-off between simulation accuracy and number of iterations required, and the authors prefer to simply adjust the limit on acceptable change in sticking coefficient over a collection of facets. There is also the option of filtering to disregard microfacets in this evaluation.

Since sticking coefficients and outgassing rates used for simulating iteration n are determined based on results of iteration $n-1$ and the time step $t(n-1)$, both parameters are slightly over-estimated for the duration $t(n)-t(n-1)$, the amount of which depends on the model being simulated. For a test case, using a limit of 10% change in sticking coefficient and 20% change in desorption rate between each iteration, the total outgassing was over-estimated by 7.67%. Lowering the limits to 1% and 5% in order to increase the temporal resolution, the difference in outgassing reduced to 1.58%. Temporal resolutions higher than 1 iteration/second could be modeled for the sticking coefficients but the main driver for a need to increase the resolution is the rate of change of desorption in the beginning of a simulation, and due to the nature of how desorption yield data is measured, data for such small doses are unreliable. Nevertheless, modification of the code to allow higher temporal resolution is possible if so desired. With suitable models for the system being simulated, additional details such as the change of desorption yield with the surface coverage, and the increase of facet temperature as function of time and SR density may be implemented to further increase the accuracy of the simulations.

6. Conclusion

The results shown here clearly demonstrate the feasibility of simulating the temporal evolution of pressure in UHV systems, taking into account both the reduction in sticking coefficient of NEG coatings and conditioning of the vacuum chambers, although the importance of having valid sticking and desorption models is clearly highlighted in the different predictions of the pressure evolution in the demonstrated case. VacuumCOST as presented here is already being utilized internally at CERN, and by external users in the framework of collaboration via the CERN knowledge transfer program, to simulate a wide range of different systems including simple pipes, gas storage cells, the insulation vacuum of hydrogen storage tanks, and beam pipe models for the FCC-ee.

Code availability

VacuumCOST is written in Python 3 and is available at https://gitlab.cern.ch/phenriks/vacuumcost. It contains a simple example model that runs out of the box to quickly get started.

An animation of the evolution of Fig. 9 from $t = 0$ is also included.

CRediT authorship contribution statement

P.L. Henriksen: Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis. **M. Ady:** Writing – review & editing, Software, Methodology. **R. Kersevan:** Writing – review & editing, Supervision, Formal analysis.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

This manuscript presents a tool developed in Python. It has been made available on GitLab and the manuscript itself contains a link under the section "Code availability".

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