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Big Data and the Dynamical Systems Approach: New Directions and Applications (chemistry, geophysical fluid dynamics) in Applied Mathematics

Stephen Wiggins, School of Mathematics

General framework and approach

Progress in applications

Requiring advances in fundamental mathematics

Resulting in new algorithms

Implemented in software

Three case studies, role of big data, motivation for new mathematical results,

1. *Intervention in environmental events in real time.*
2. *Autonomous underwater vehicle mission planning.*
3. *Lagrangian transport in the Arctic ocean.*
4. *Adoption of our methods and approach in chemistry*
5. *KAM and Nekhoroshev Theorems for aperiodically time dependent Hamiltonian systems*

Lagrangian transport in geophysical flows: The Dynamical Systems Approach

S. Wiggins, The dynamical systems approach to Lagrangian transport in oceanic flows. Annu. Rev. Fluid. Mech., 37, 295-328 (2005).

Applications force the need to develop theoretical and computational Techniques for dynamical systems with aperiodic time dependence

Two broad categories of “types of results”

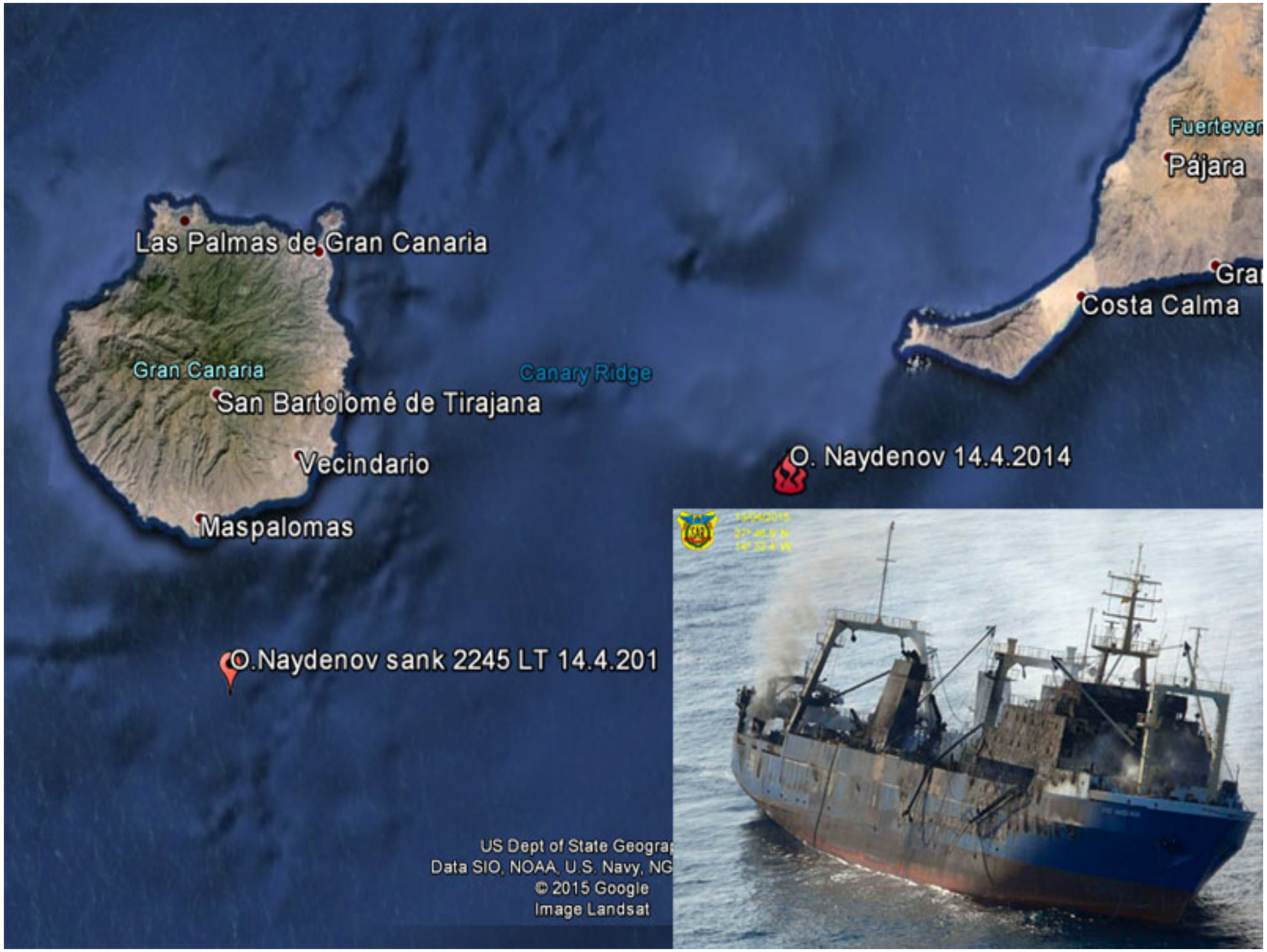
Hyperbolic (nature of time dependence is, generally, not essential)

e.g. hyperbolic trajectories, Stable and unstable manifolds, chaos

Elliptic (nature of time dependence is absolutely essential)

e.g. KAM Theorem, Nekhoroshev’s Theorem

Case Study 1:The Strange Saga of the Oleg Naydenov



Brief Summary of Events

TIMELINE

11/4/2015—Fire breaks out

14/4/2015—Ship towed away and sunk

16/4/2015—Oil slicks spotted on the surface

23/4/2015—Oil reaches Gran Canaria

Immediate Need: Predict "What will happen?"

V. J. García-Garrido, A. Ramos, A. M. Mancho, J. Coca, and S. Wiggins, A dynamical systems perspective for a real-time response to a marine oil spill. Marine Pollution Bulletin. 112, 201-210 (2016).

Data:

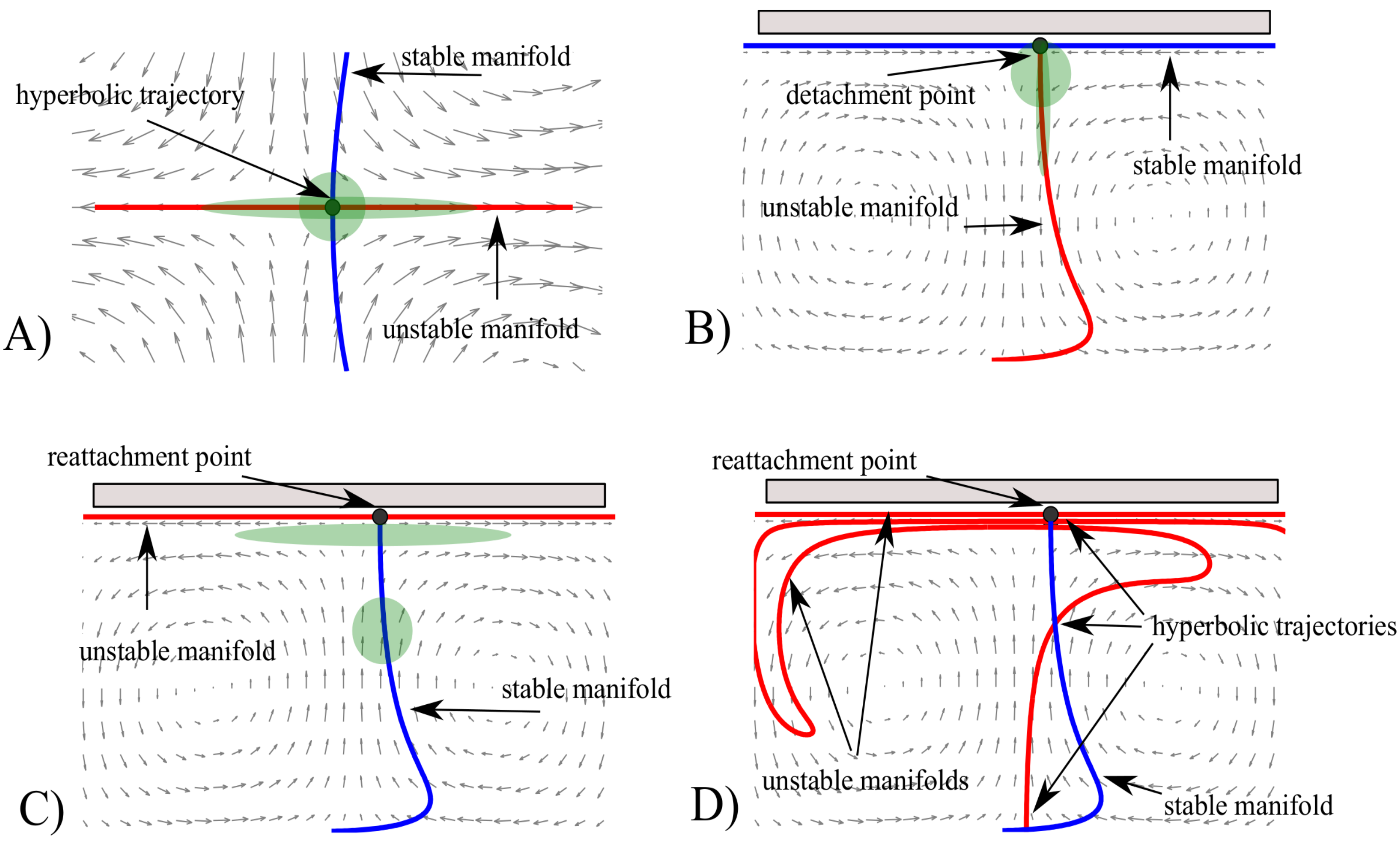
in-situ observations (aircraft, ships)
satellite observations
testimony of people in the affected area

Mathematical Modelling and Analysis:

Copernicus Marine Environment Monitoring Service (CMEMS)
Provides high resolution velocity fields, 5 day predictive window

European Commission
COPERNICUS
MARINE ENVIRONMENT MONITORING SERVICE
Providing PRODUCTS and SERVICES for all marine applications

Lagrangian Template: Concepts from Dynamical Systems Theory



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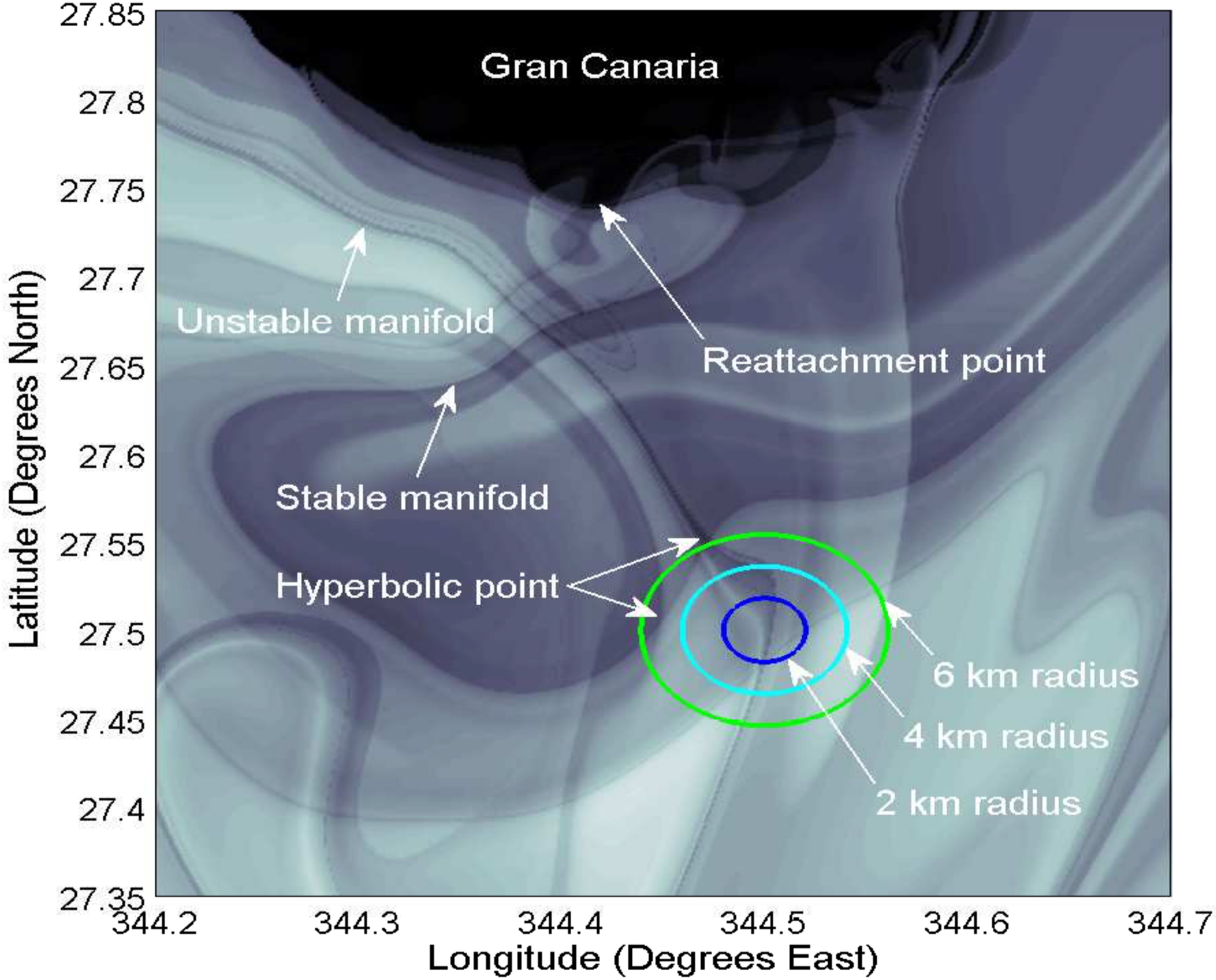
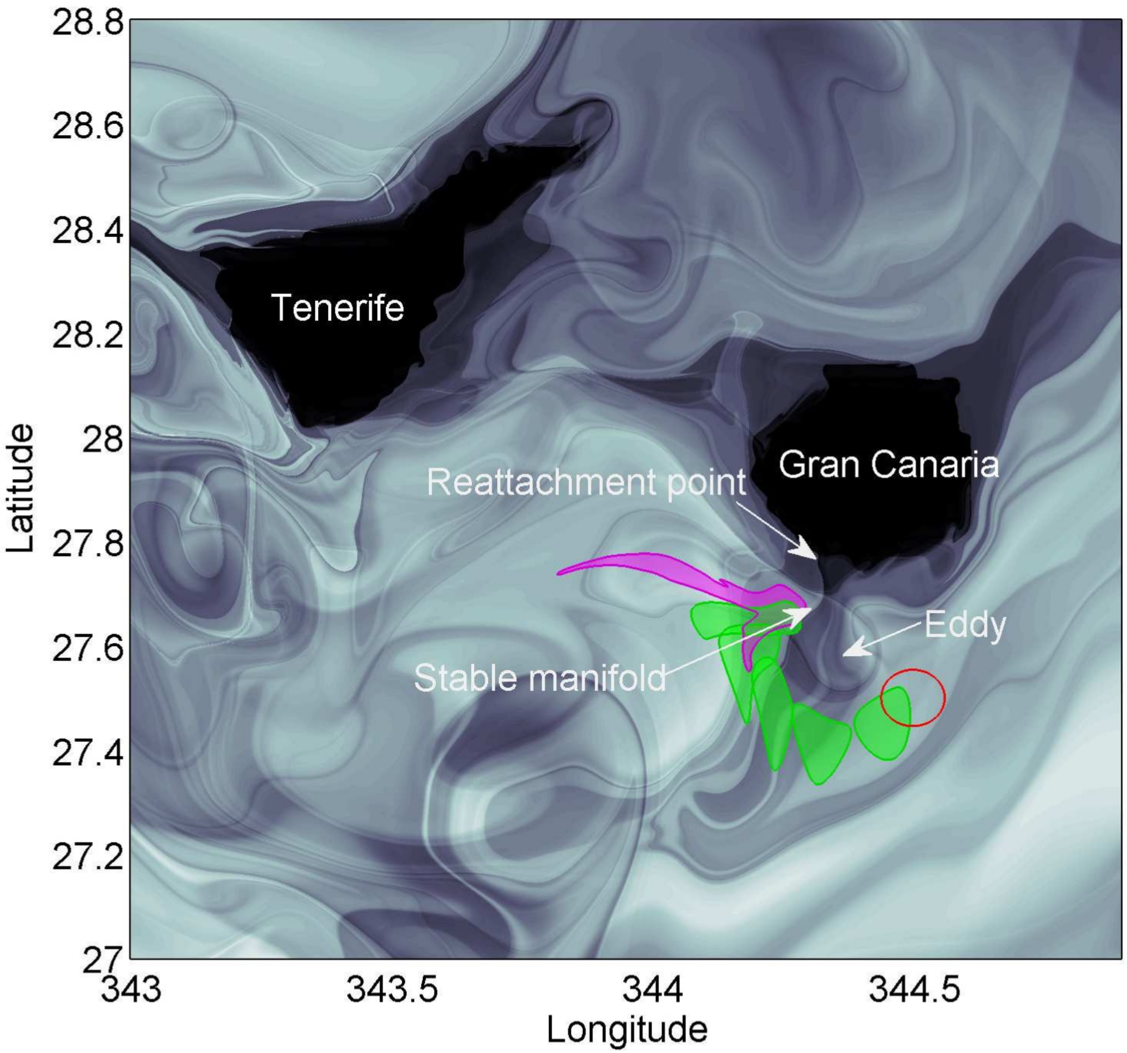
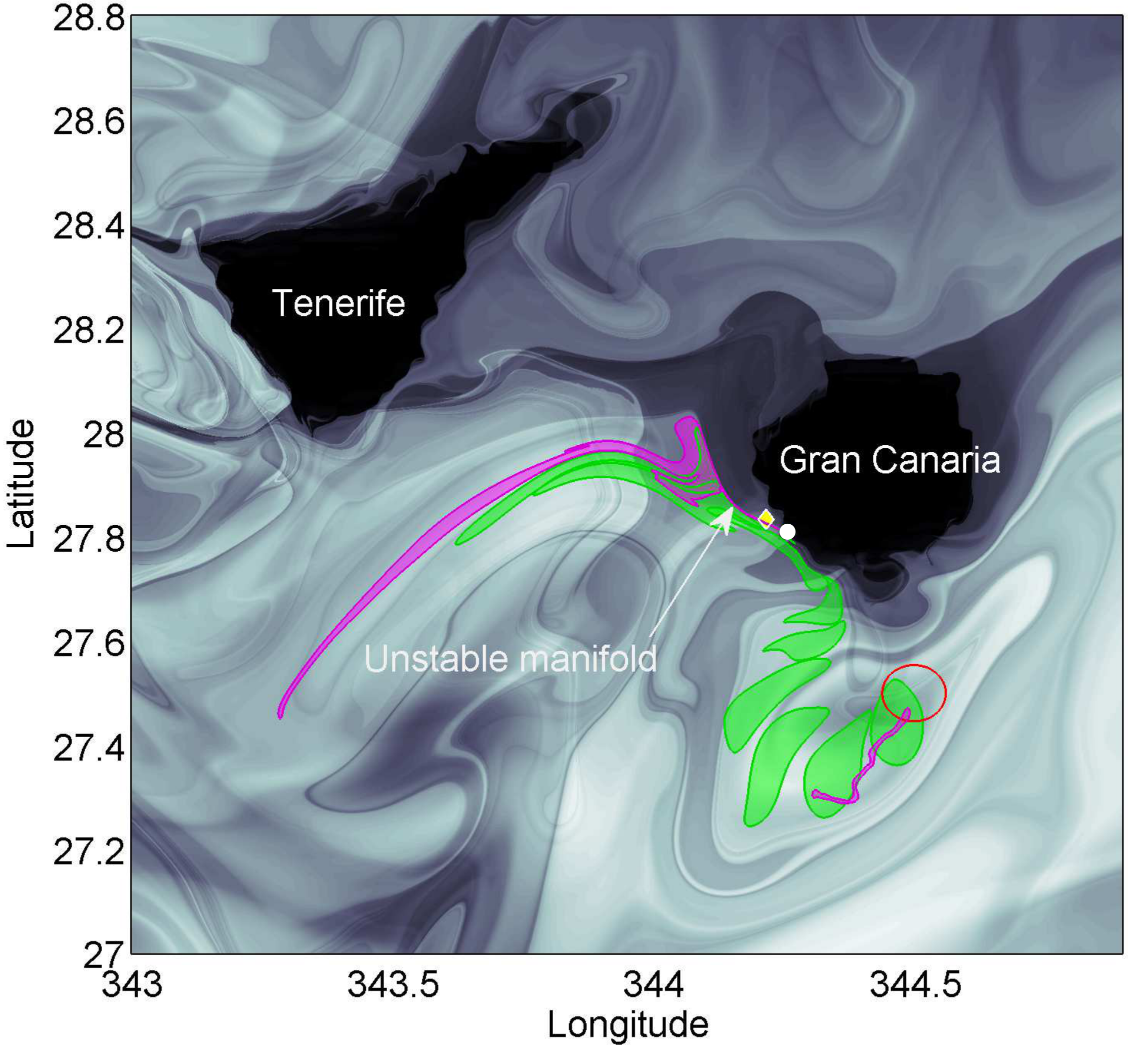

Gran Canaria
Unstable manifold
Reattachment point
Stable manifold
Hyperbolic point
6 km radius
4 km radius
2 km radius
Latitude (Degrees North)
Longitude (Degrees East)
27.85
27.8
27.75
27.7
27.65
27.6
27.55
27.5
27.45
27.4
27.35
344.2
344.3
344.4
344.5
344.6
344.7

April 15


28.8
28.6
28.4
28.2
28
27.8
27.6
27.4
27.2
27
Latitude
343
343.5
344
344.5
Longitude
Tenerife
Gran Canaria
Reattachment point
Stable manifold
Eddy

19 April



23 April

We predicted the day and location that the spill reached land

Case Study 2: The Trans-Atlantic Journey of Silbo-The Glider

A.G. Ramos, V. J. García-Garrido, A. M. Mancho, S.Wiggins, J. Coca, S. Glenn, O. Schofield, J. Kohut, D. Aragon, J. Kerfoot, T. Haskins, T. Miles, C. Haldeman, N. Strandskov, B. Allsup, C. Jones, and J. Shapiro.
<u>Lagrangian coherent structure assisted path planning for transoceanic autonomous underwater vehicle missions.</u>
Scientific Reports. ***8****, 4575 (2018).*

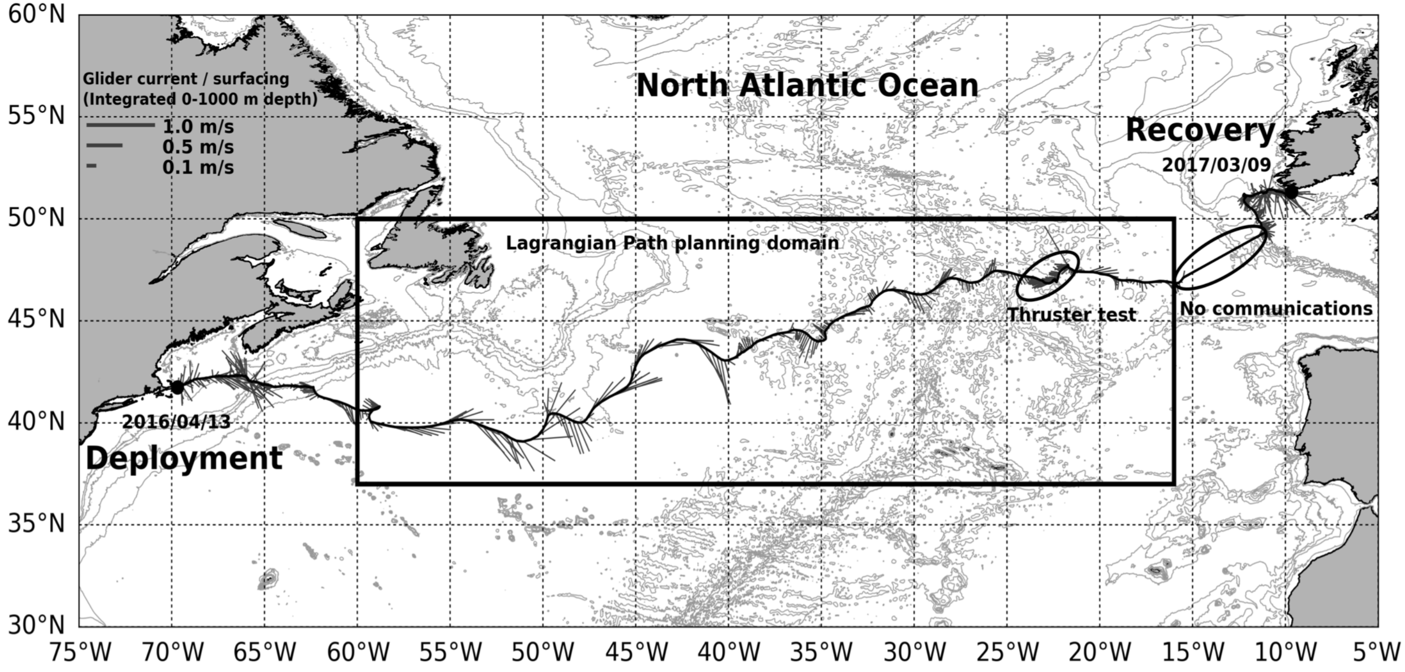
Deployed: 13/4/2016 (Falmouth, MA)

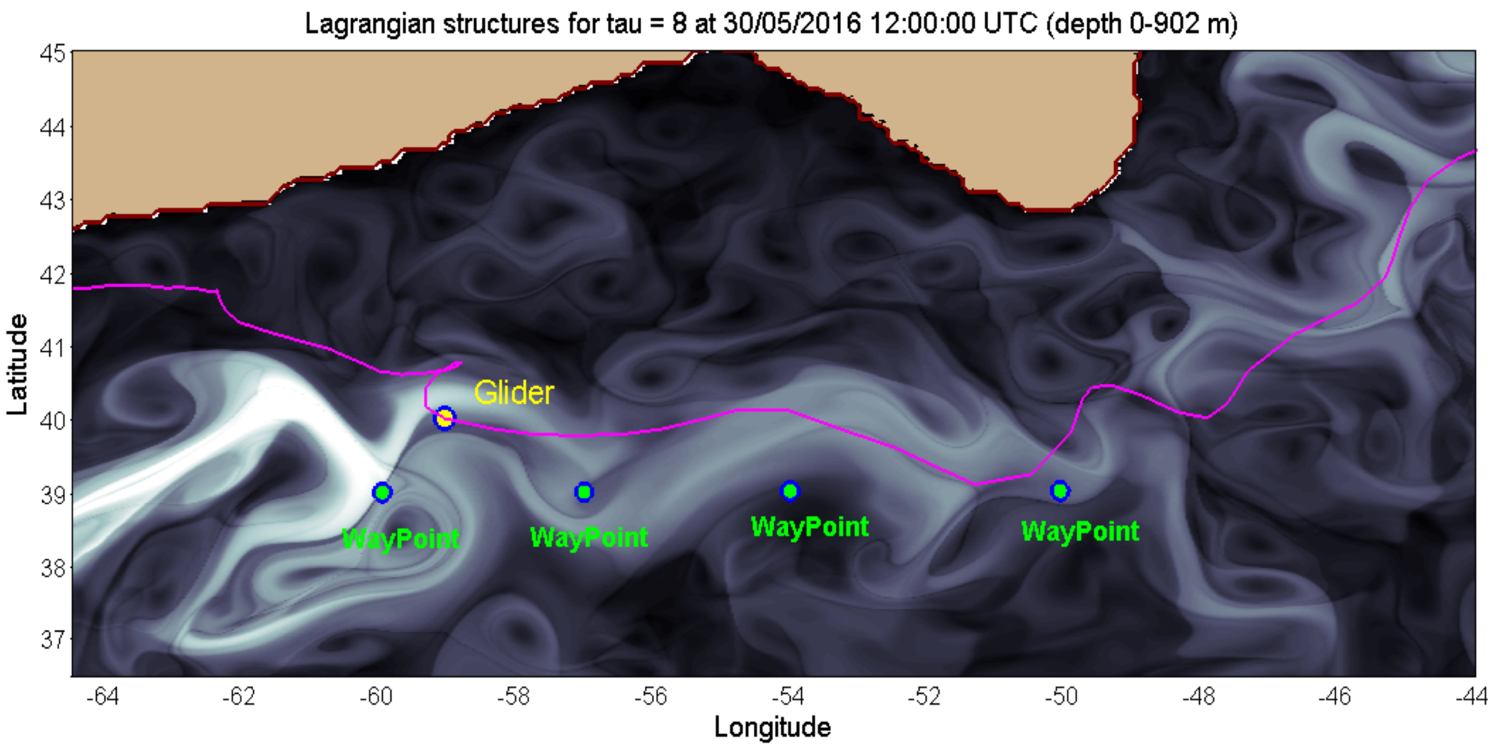
Recovered: 9/3/2017 (South of Ireland)

6506 km journey

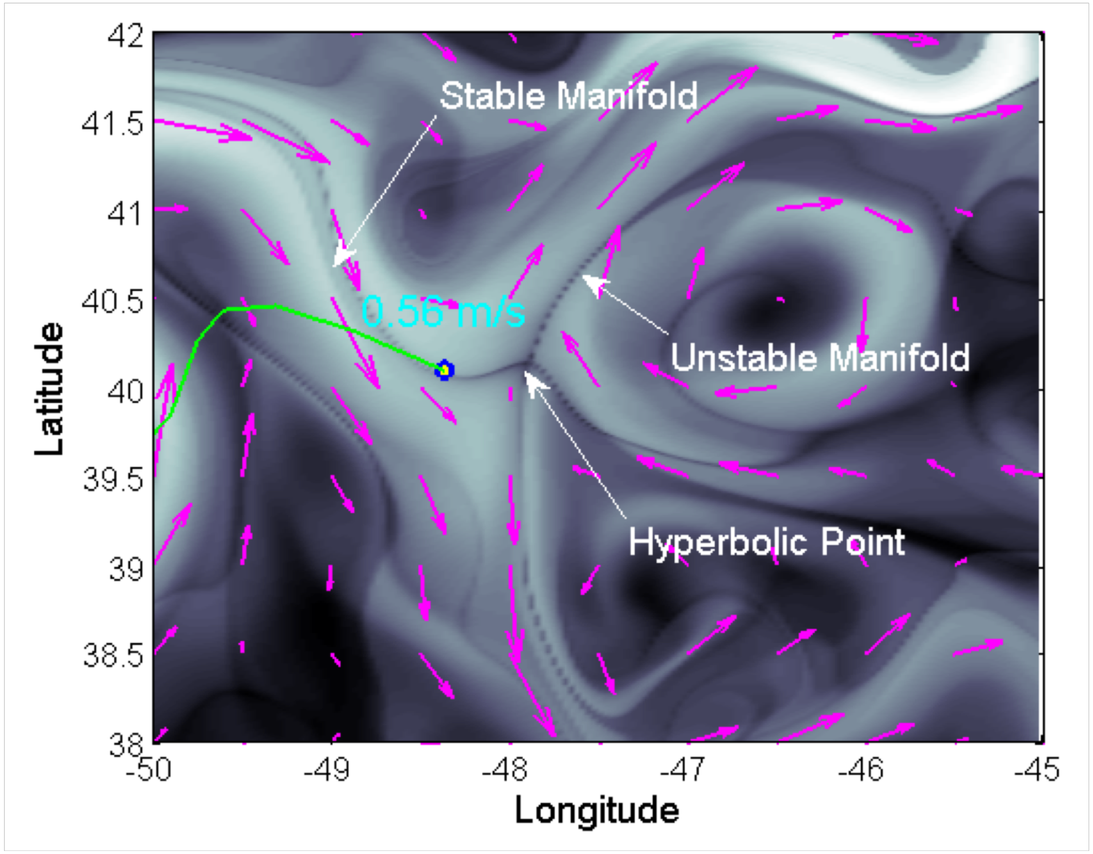
Consumed all of its lithium batteries (equivalent energy of less than a liter of gasoline)

The Route

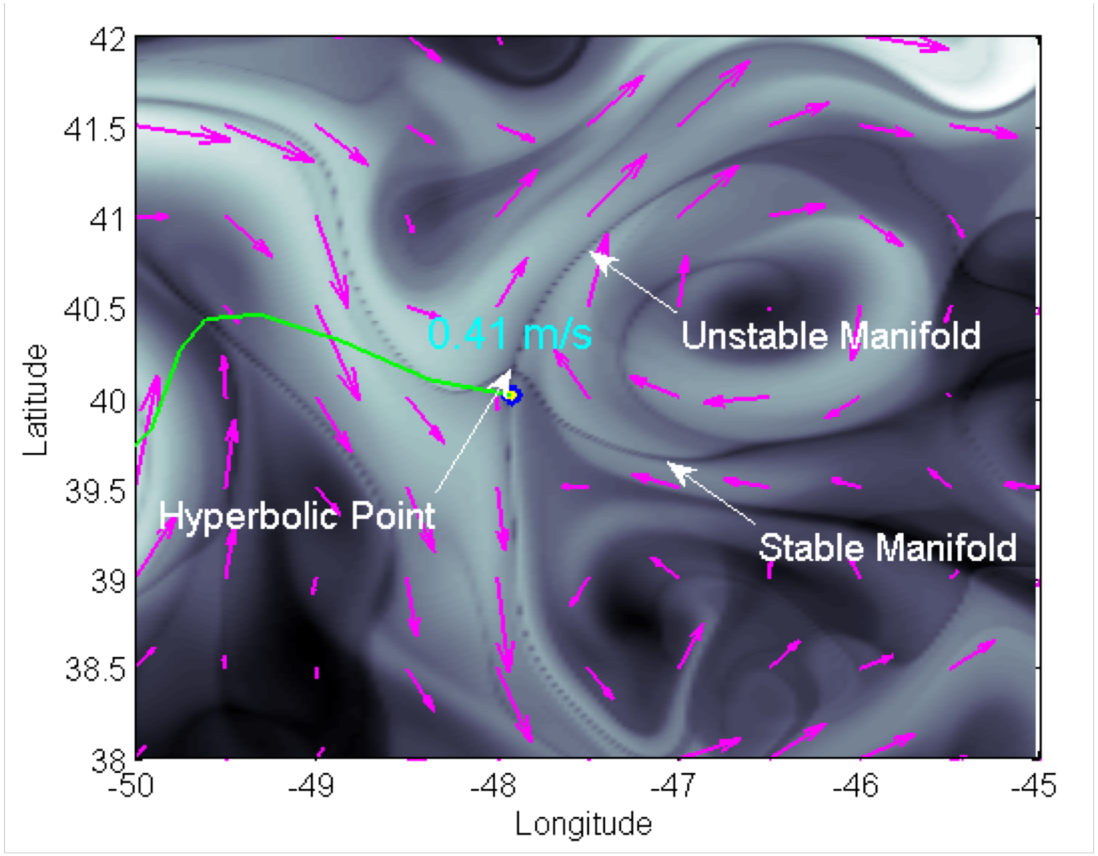

North Atlantic Ocean
Glider current / surfacing
(Integrated 0-1000 m depth)
1.0 m/s
0.5 m/s
0.1 m/s
Lagrangian Path planning domain
Recovery
2017/03/09
Thruster test
No communications
2016/04/13
Deployment
60°N
55°N
50°N
45°N
40°N
35°N
30°N
75°W
70°W
65°W
60°W
55°W
50°W
45°W
40°W
35°W
30°W
25°W
20°W
15°W
10°W
5°W



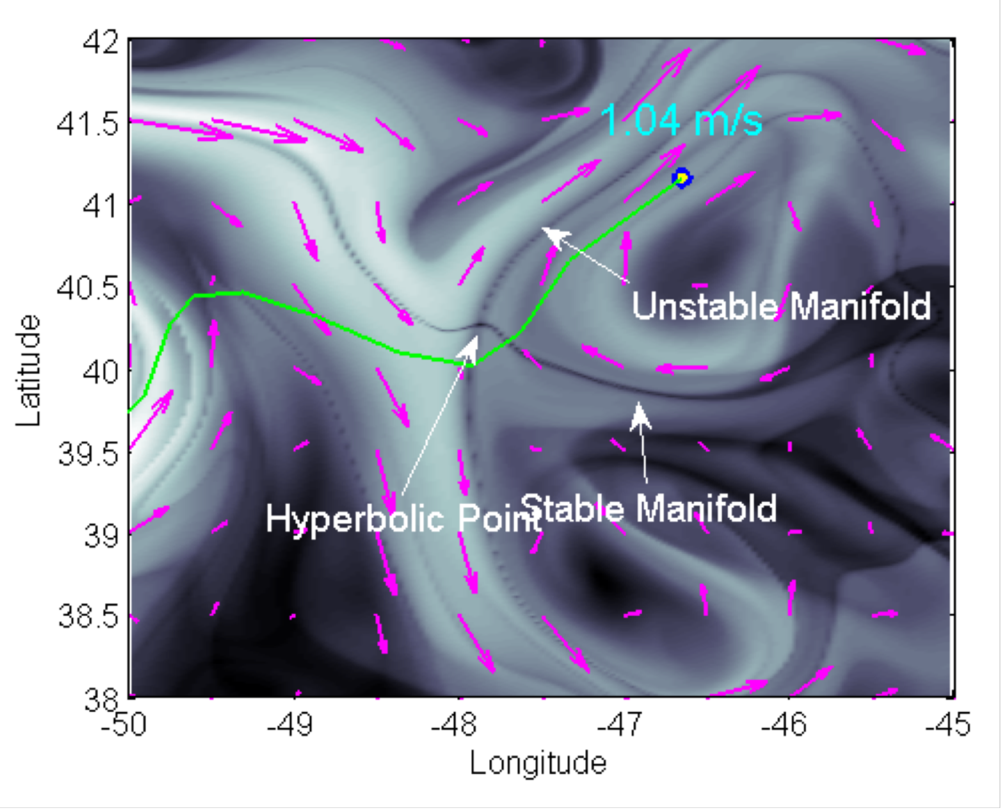
Lagrangian structures for tau = 8 at 30/05/2016 12:00:00 UTC (depth 0-902 m)
Glider
WayPoint
WayPoint
WayPoint
WayPoint
Latitude
Longitude
45
44
43
42
41
40
39
38
37
-64
-62
-60
-58
-56
-54
-52
-50
-48
-46
-44



19th June 2016



20th June 2016



23rd June 2016

Record speed!

Case Study 3: Lagrangian Transport in the Arctic Ocean

F. Balibrea-Iniesta, J. Xie, V. J. Garcia-Garrido, L. Bertino,A. M. Mancho, and S.Wiggins, Lagrangian transport across the upper Arctic waters in the Canadian Basin, *Quarterly Journal of the Royal Meteorological Society*, **145** (718) Part A, 76-91 (2019).

The present work uses of ocean velocity and salinity fields distributed by the Copernicus Marine Environment Monitoring Service. These data are integrated into a product called ``Arctic Ocean Physics Analysis and Forecast''
and are downloadable from http://marine.copernicus.eu.

This product is based on the TOPAZ4 numerical prediction system, which is an operational real time ocean monitoring and forecast system covering the North Atlantic and Arctic Oceans with a resolution of 12.5 km. TOPAZ4 was developed and is maintained by NERSC. It is composed of a previous circulation model called HYCOM coupled to a sea-ice model due and three ecosystem models of increasing complexity.

The TOPAZ4 production cycle is run on a weekly basis, starting with a data assimilation step which is completed with a one-week simulation run to produce a best estimate for each of the preceding 7 days. Finally, a 10-day forecast is run daily using the most recent analysis, forced by updated and perturbed atmospheric fields.

Data is supplied daily at 10 different layer depths, varying from 5 m to 1000 m depth and a spatial resolution of 12.5 km.

Our work is for **2013-2015**

at **30 m depth**

Goal: Characterize the “major currents” (e.g. the Beaufort gyre and the Transpolar Drift) in a *dynamical Lagrangian sense* so as to predict their interaction, e.g. do they influence each others evolution, and their infuence on transport e.g. are they barriers or mixers where and when do they move particles

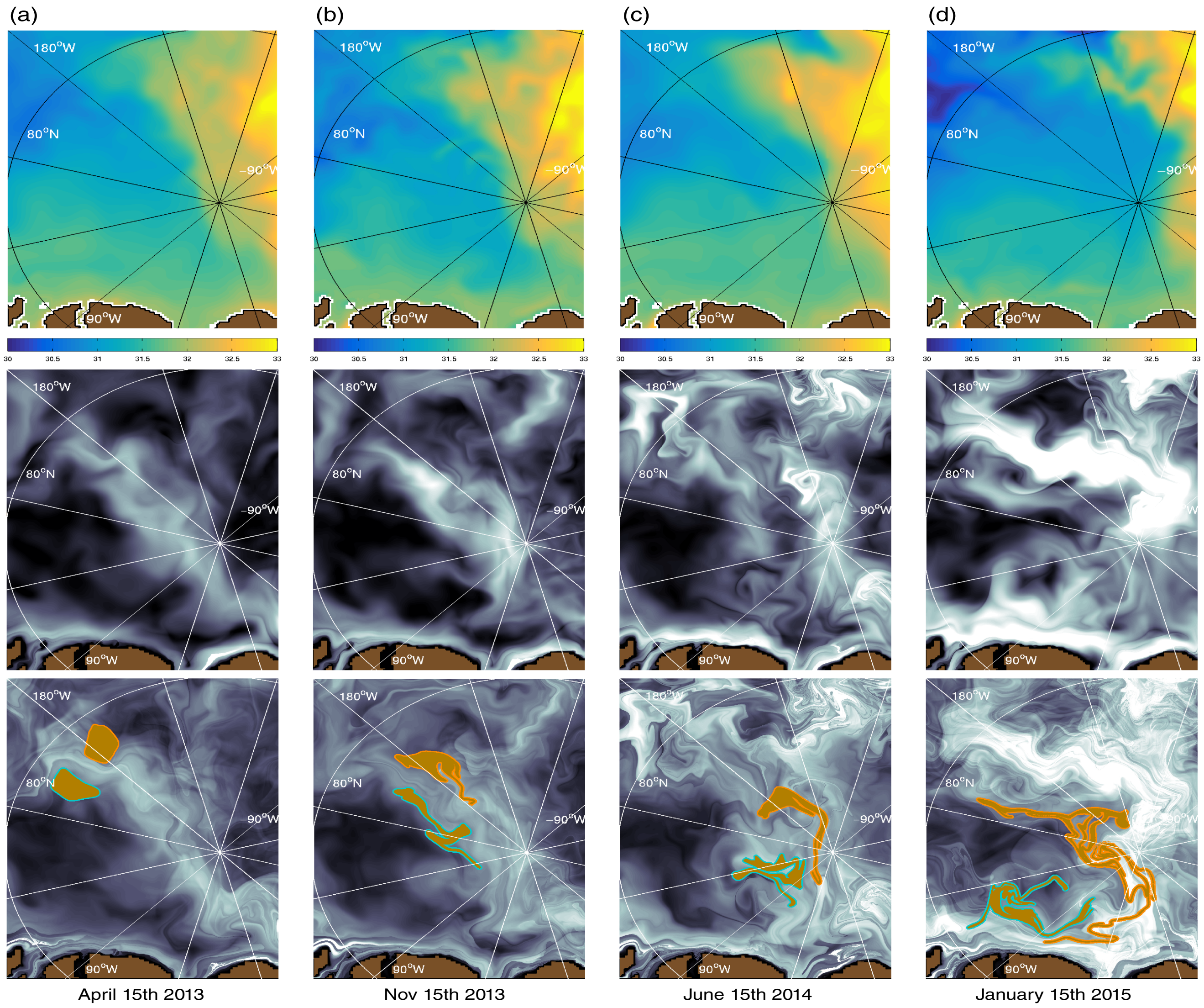


FIGURE 13 In the upper row, the panels represent salinity (parts per thousand) on four different dates: (a) April 15, 2013, (b) November 15, 2013, (c) June 15, 2014 and (d) January 15, 2015. The colourbar ranges from 30 to 33 psu of salinity. The second and third rows represent the function M calculated with $\tau = 100$ and $\tau = 300$ days, respectively. The bottom row indicates two blobs of water particles depicted in orange on either side of the TDS, which are then advected through the panels [Colour figure can be viewed at wileyonlinelibrary.com]

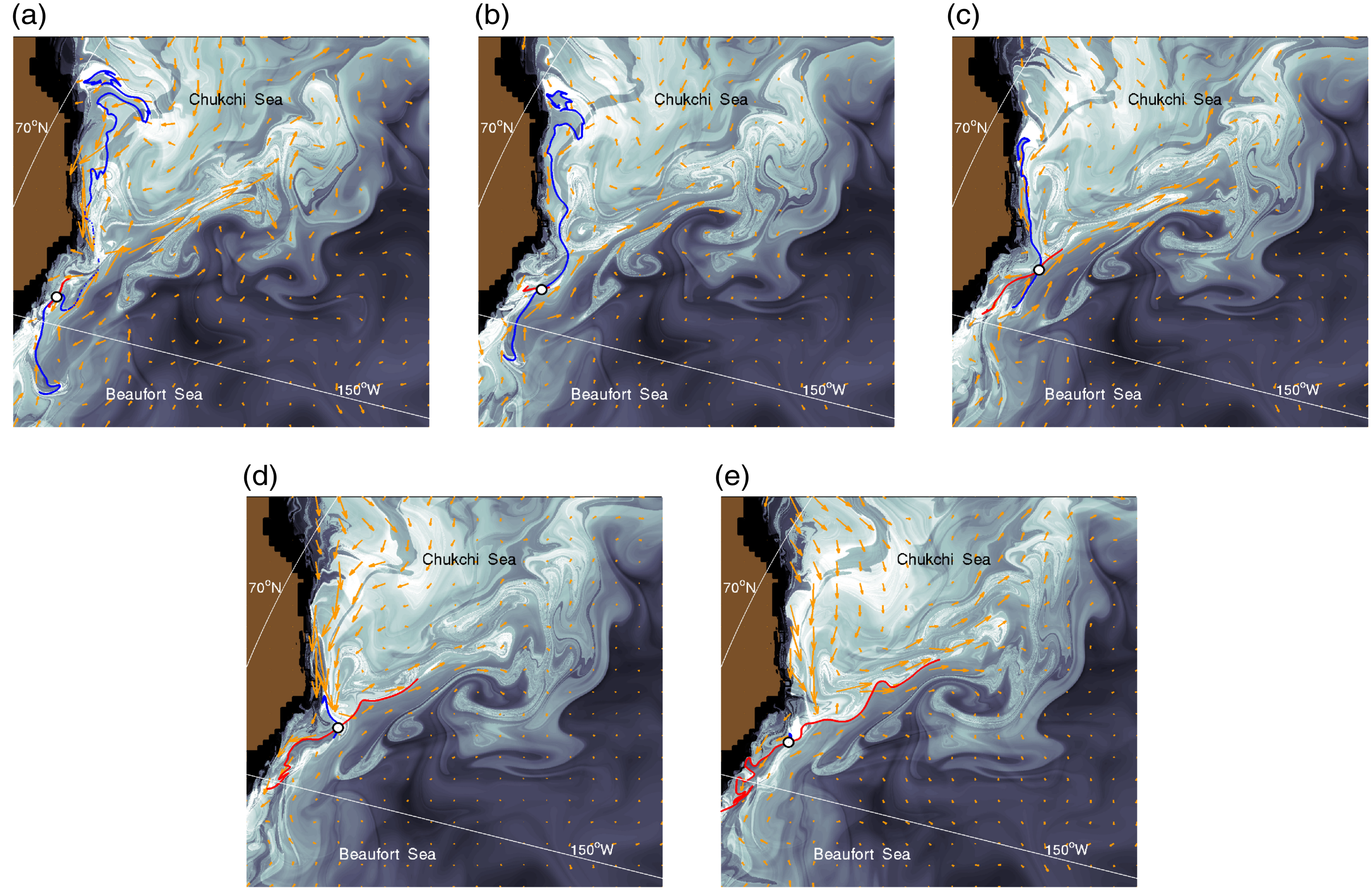
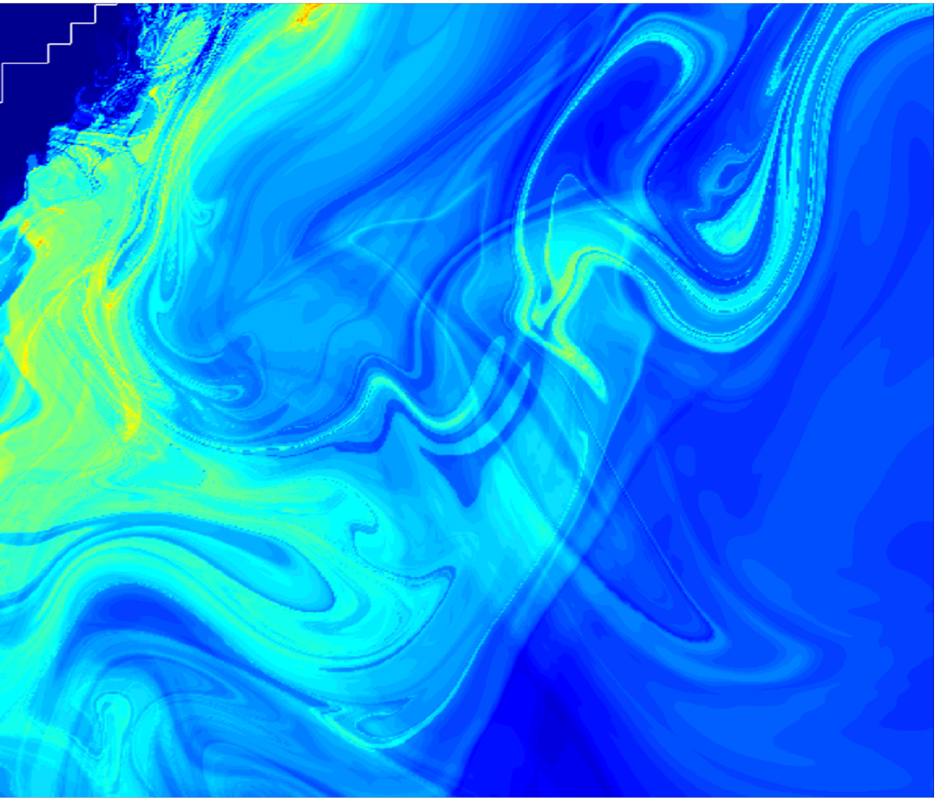


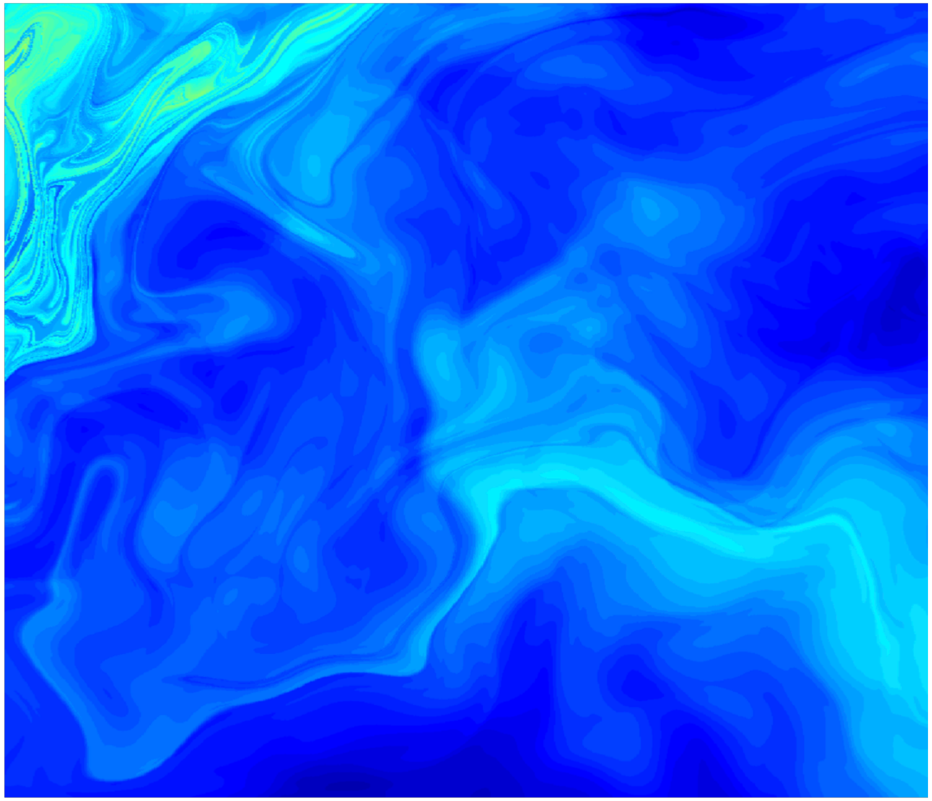
FIGURE 8 The configuration of a detachment point on the Arctic coastline, highlighted by means of the function M. The white dot highlights the hyperbolic trajectory and the red and blue curves denote, respectively, the unstable and stable manifolds. The velocity field is overlaid. (a) October 1, 2013; (b) October 15, 2013; (c) November 1, 2013; (d) November 15, 2013; (e) December 1, 2013 [Colour figure can be viewed at wileyonlinelibrary.com]

Two Selected Locations of the Beaufort Gyre

Region of strong mixing (anti-cyclonic)



Region of the Canada Basin, where the main branch of the TDS emerges



How are these flow structures revealed ? ***Method of Lagrangian Descriptors***

A.M. Mancho, S. Wiggins, J. Curbelo, C. Mendoza Lagrangian descriptors: A method for revealing phase space structures of general time dependent dynamical systems, *Communications in Nonlinear Science and Numerical Simulation*, **18(**12), 3530 – 3557 (2013).

C. Mendoza, A. M. Mancho and S. Wiggins, Lagrangian Descriptors and the Assessment of the Predictive Capacity of Oceanic Data Sets. *Nonlinear Processes in Geophysics*, **21**, 677-689 (2014).

C. Lopesino, F. Balibrea -Iniesta, S. Wiggins, and A. M. Mancho, Lagrangian descriptors f or two dimensional, area preserving, autonomous and nonautonomous maps, *Communications in Nonlinear Science and Numerical Simulation*, **27**, 40–51 (2015).

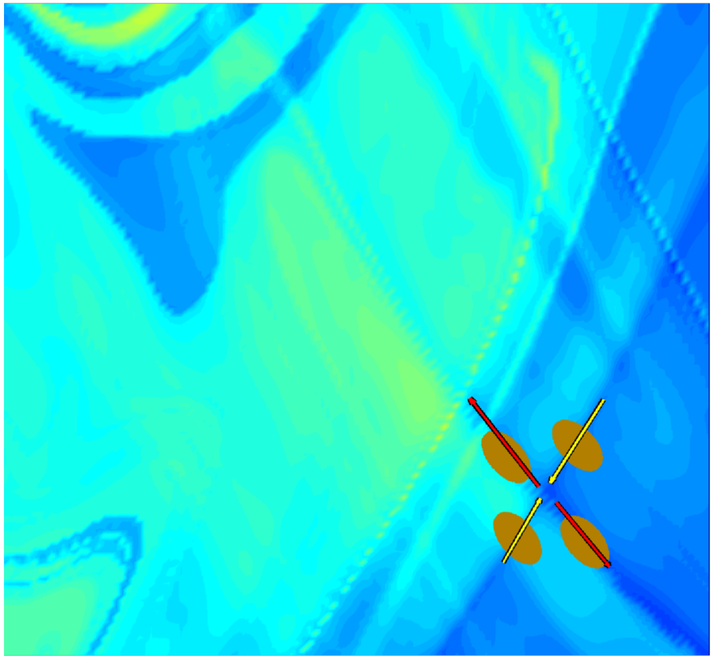
F. Balibrea-Iniesta, C. Lopesino, S. Wiggins, and A. M. Mancho, Lagrangian Descriptors for Stochastic Differential Equations: A Tool for Revealing the Phase Portrait of Stochastic Dynamical Systems. *International Journal of Bifurcation and Chaos*, **26**(13), 1630036 (2016).

C. Lopesino, F. Balibrea-Iniesta, V. J. Garcia-Garrido, S. Wiggins, and A. M. Mancho, A theoretical Framework for Lagrangian descriptors. *International Journal of Bifurcation and Chaos*, **27**(1), 1730001 (2017).

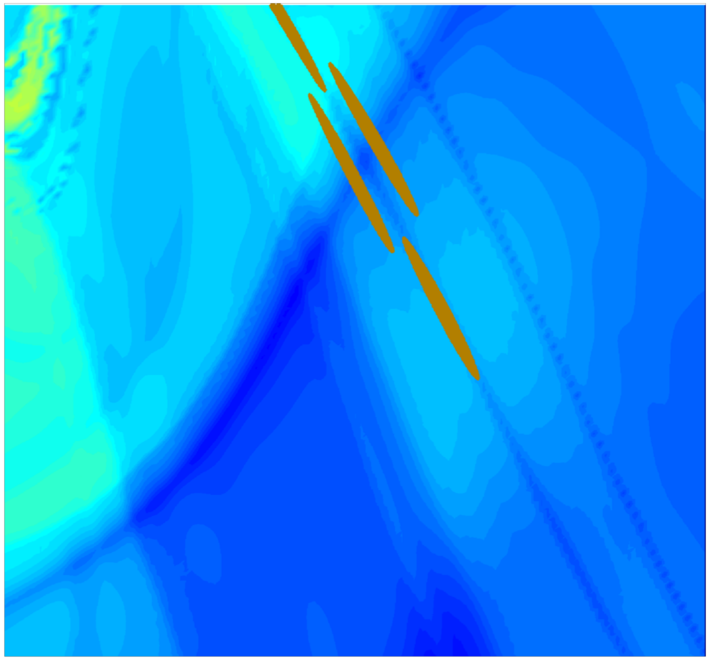
Choose initial time, t_0. Fix $\tau > 0$.

For every x_0 in the region of interest, compute the arclength through x_0 for the time Interval $[t_0 - \tau, \; t_0 + \tau]$. Denote the field of arclengths by:

$M(x_0\,;\; t_0, \tau)$ -- A Lagrangian Descriptor



1 April 2013



1 July 2013

"singular curves" of $M(x_0\,;\; t_0, \tau)$ are aligned with invariant curves. Crossings of singular curves correspond to hyperbolic trajectories

Two points

These three topics (Oleg Naydenov, Silbo the glider, Arctic Ocean transport) collectively provide predictive analysis strategies for future important problems, e.g. glider missions across the Arctic ocean are being considered, and there will be drilling for oil in the Arctic region. ***New capabilities: significant broad interest***

Fundamentally, the topic of Lagrangian transport in fluid mechanics is a subset of the general topic of the geometry of transport in phase space

Similarly, this point of view has many implications and applications In science and engineering, in general

A recent “transition”: New developments in chemistry

G. T. Craven and R. Hernandez, "Lagrangian descriptors of thermalized transition states on time-varying energy surfaces," *Phys. Rev. Let.* **115**, 148301 (2015).

A.Junginger and R. Hernandez, "Uncovering the geometry of barrierless reactions using Lagrangian descriptors," *J. Phys. Chem. B*, **120**, 1720 (2016). (In the Bruce C. Garrett Festschrift issue, March 2, 2016.)

A.Junginger and R. Hernandez, "Lagrangian descriptors in dissipative systems," *Phys. Chem. Chem. Phys.* **18**, 30282 (2016).

A,Junginger, L. Duvenbeck, M. Feldmaier, J. Main, G. Wunner, and R. Hernandez. “Chemical dynamics between wells across a time-dependent barrier: Self-similarity in the Lagrangian descriptor and reactive basins”. *J. Chem. Phys.,* **147,** 064101 (2017).

P. Schraft, A. Junginger, M. Feldmaier, R. Bardakcioglu, J. Main, G. Wunner, R. Hernandez Neural network approach to time-dependent dividing surfaces in classical reaction dynamics, *Phys. Rev. E*, **97**, 042309 (2018)

Rapidly developing experimental techniques → Reassessment of Traditional models and methodologies → Leading to the development of a new mathematical area of research: ***Phase Space Chemistry***

The Discovery of "Roaming" as a dynamical mechanism for chemical reaction

J. M. Bowman and A. G. Suits, Roaming Reactions :The Third Way, *Physics Today*, **64**(11), 33 (2011) .


Roaming reactions: The third way

Joel M. Bowman and Arthur G. Suits

Chemists have long held that there are two ways in which a molecule can break apart. But recent results show a third possibility, and its discovery may have far-reaching implications.

Why does formaldehyde "roam" and not "dissociate"?

F. A. L. Mauguiere, P. Collins, Z. C. Cramer, B. K. Carpenter, G.S. Ezra, S. C. Farantos, and S. Wiggins, Phase space structures explain hydrogen atom roaming in formaldehyde decomposition. *Journal of Physical Chemistry Letters*, **6**(20), 4123–4128 (2015).

Resulting in the following invited review paper.

F. A. L. Mauguiere, P. Collins, Z. C. Kramer, B. K. Carpenter, G.S. Ezra, S. C. Farantos, and S. Wiggins, Roaming: A Phase Space Perspective. *Annual Review of Physical Chemistry*, **6**8, 499-524 (2017).

Chemists have recognized the tremendous scope and need for mathematics, but can mathematicians contribute?

Recently, we have been given the *task and resources* to develop the new field of ***Phase Space Chemistry***

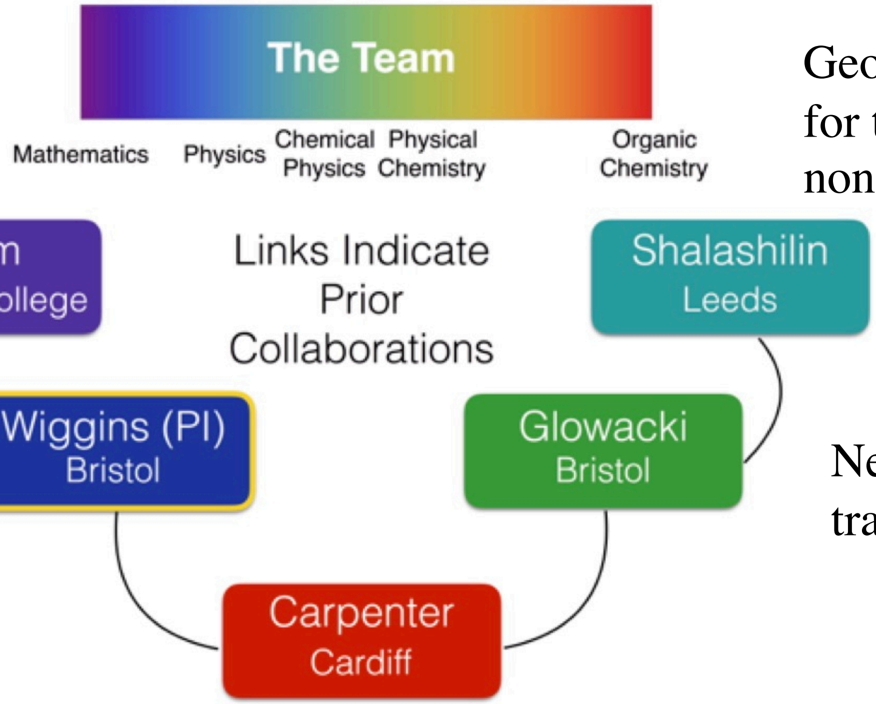
Chemistry and Mathematics in Phase Space

EPSRC-Funded Programme Grant: 2017-2023

5 million £, 36 person-years of postdoctoral support

Geometric classical and quantum mechanics

Geometrical methods for trajectory guided non-adiabatic dynamics



Development of the geometrical structure of phase space transport for reaction dynamics

New concepts in trajectory analysis

System-bath modeling

All areas of applications that generate "lots of trajectories" (Big Data) must embrace ***Machine Learning Methodology—The Future***

(Revealing patterns and structure in trajectory data sets: this is the Dynamical systems point of view.)

Empirical Classification of Trajectory Data: An Opportunity for the Use of Machine Learning in Molecular Dynamics

Barry K. Carpenter, Gregory S. Ezra, Stavros C. Farantos, Zeb C. Kramer, Stephen Wiggins

J. Phys. Chem. B, **2018**, *122* (13), pp 3230–3241
DOI: 10.1021/acs.jpcb.7b08707
Publication Date (Web): October 2, 2017

KEYWORDS: Machine learning, dynamics, periodic orbit, roaming.

Future Work and Issues

Future work: The Arctic, Continue to develop the mathematics that leads to real time and operational capabilities (a rigorous theory for Lagrangian descriptors), Merging machine learning and dynamical systems methodologies—applications and rigorous foundations. Develop the new field of "Phase Space Chemistry".

Keep and eye out for, and take advantage of, new opportunities that arise.Applied Mathematics should be a ***dynamic subject***

Issues: *Human resources*. Educating applied mathematicians with the necessary skills needed to tackle 21st century applications (e.g. quantum mechanics) with expertise in applied and computational dynamical systems, applied statistics as well as "useful" computational skills and expertise for dealing with data sets.

New KAM and Nekhoroshev Theorems for Aperiodic Time Dependence

*New approaches, and mathematics, required to deal with the issue that **time is not compact**.*

A. Fortunati and S. Wiggins, Normal form and Nekhoroshev stability for nearly integrable Hamiltonian systems with unconditionally slow aperiodic time dependence, *Regular and Chaotic Dynamics*, **19**(3), 363-373 (2014).

A. Fortunati and S. Wiggins, Persistence of Diophantine Flows for Quadratic Nearly Integrable Hamiltonians under Slowly Decaying Aperiodic Time Dependence, *Regular and Chaotic Dynamics*, **19**(5), 586-600 (2014).

A. Fortunati and S. Wiggins, A Kolmogorov Theorem for Nearly Integrable Poisson Systems with Asymptotically Decaying Time-dependent Perturbation, *Regular and Chaotic Dynamics*, **20**(4), 476-485 (2015).

A.Fortunati and S. Wiggins. Negligibility of small divisor effects in the normal form theory for nearly-integrable Hamiltonians with decaying non-autonomous perturbations. *Celestial Mechanics and Dynamical Astronomy,* **125**(2), 247-262 (2016).

A. Fortunati and S. Wiggins, Normal forms *à la Moser* for aperiodically time-dependent Hamiltonians in the vicinity of a hyperbolic equilibrium. *Discrete and Continuous Dynamical Systems-S,* **9** (4), 1109-1118 (2016).

A. Fortunati and S. Wiggins, Integrability and strong normal forms for non-autonomous systems in a neighbourhood of an equilibrium, *Journal of Mathematical Physics*, **57**, 092703 (2016).