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Robust and accurate approximation of hyperbolic systems

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14. ABSTRACT
Research objectives: The project consists of developing robust numerical methods for solving hyperbolic systems of conservation laws such as the compressible Euler equations and radiative hydrodynamics. Most current high-order numerical methods are unattractive to practitioners because they are not robust. Our research program consists of developing numerical methods with the following properties, all related to robustness: (i) be invariant domain preserving on any unstructured meshes in any space dimension; (ii) do not involve any tuning parameters, mesh-dependent or problem-dependent stabilizations (no subtle mathematical knowledge should be required from practitioners to use these methods); (iii) be at least third-order accurate in space and time and be open to higher-order extensions; (iv) be consistent with physical dissipation mechanisms. The above objectives will be reached by stating precise statements supported either by mathematical proofs or very strong numerical evidences. Technical approaches: We propose to use the first-order invariant domain preserving method we have developed in the previous grant period as a robust basis for a highorder method constructed by adding a dissipation proportional to the local violation of the second-principle of thermodynamics. Since all high-order techniques develop un-physical oscillations (by Godunov's theorem), we are going to correct these oscillations by identifying a proper local admissible convex domain where the solution must stay.

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1 Accomplishments

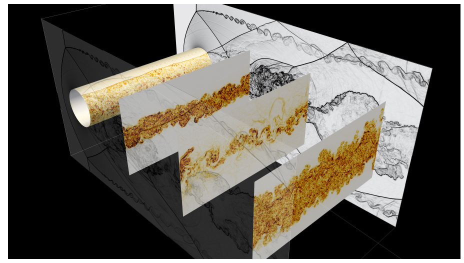
The objective of the 2018-2021 project was to develop robust numerical methods for solving hyperbolic systems of conservation laws such as the Euler equations, the shallow water equations, and related systems such as radiative hydrodynamics. The emphasis was put on robustness.
Thirteen scientific papers have been published in the context of the grant. The major results obtained during the award period are the following:

New stability results for nonlinear hyperbolic systems: We have constructed a robust numerical method to approximate general hyperbolic systems in any space dimension using forward Euler time stepping and finite elements on non-uniform grids. The method is discretization agnostic: it works with continuous and discontinuous finite elements. The invariant domain property is proved to hold for any hyperbolic system provided a standard CFL condition holds. The solution is also shown to satisfy a discrete entropy inequality for every admissible entropy of the system. The method is formally first-order accurate in space and can be made high-order in time by using strong stability preserving algorithms. This breakthrough result has no analog in the continuous finite element literature. We have developed a computationally efficient algorithm in the context of the Euler system of gas dynamics with the co-volume equation of state. The technique has been extended to the Arbitrary Lagrangian Eulerian (ALE) framework, Guermond et al. [6, 11] and the shallow water equations Azerad et al. [1]. We have also extended the theory to dispersive equations like the Serre-Green-Naghdi equations Guermond et al. [17], Guermond et al. [16]. Since Suliciu approximate Riemann solvers are popular in the literature, we have investigated some properties of these method and have proved that these methods are not robust (even the first-order ones). Counterexamples are provided in Guermond et al. [10].

Scalar equations: High-order maximum principle preserving methods. To make the robust method described above more accurate for time-dependent scalar conservation equations, we have developed in Guermond and Popov [4] a new class of maximum principle preserving methods. In this case the invariant domain property reduces to the local maximum principle which essentially amounts to enforcing linear constraints. This can be done by using the flux corrected transport (FCT) methodology. We have also developed an anti-diffusive technique for the level set method in Guermond et al. [5]. We have analyzed the effect of the use of the consistent mass matrix on the maximum principle in Guermond et al. [7] and have shown that it is not possible to achieve strict maximum principle unless the mass matrix is lumped. These results are valid for arbitrary nonlinear scalar conservation equations.

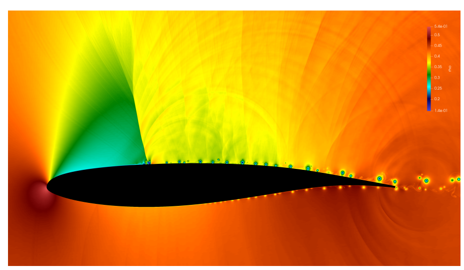
Hyperbolic systems: Convex limiting: Extending the method described in [4] to hyperbolic systems has been a long dry process with many dead ends. For instance the standard flux corrected transport technique cannot be used for hyperbolic systems since the invariant domain is a convex set whose boundary is not a finite intersection of hyperplanes (recall that FCT is based on linear functionals since the method amounts to grouping positive fluxes and negative fluxes together). After many setbacks we made a nontrivial breakthrough in 2018. In collaboration with I. Tomas (then postdoc at TAMU mentored by the PIs), we proposed in Guermond et al. [8, 12] a new way to enforce nonlinear constraints which we coined “convex limiting”. In the spirit of the FCT method, the idea consists of blending the robust first-order invariant domain preserving technique with a higher-order method that conserves the same mass. The sum of the high-order and low-order flux differences is decomposed into a convex combination, and each member of this sum is limited by using a line search that is guaranteed to have a unique solution. This technique can be used to enforce any constraint based on a quasi-concave (or quasi-convex) functional. Another very important feature of this technique is that for each quasi-concave functional, the PI have developed local bounds that are guaranteed to be inside the invariant set. These bounds are based on a fundamental new result proved in Guermond and Popov [3] for the robust invariant domain preserving low-order method. The method is agnostic to the type of the hyperbolic system. It is illustrated in Guermond et al. [8] for the compressible Euler system. We have extended the convex limiting technique to finite volume schemes called "central schemes" in Popov and Hua [21]. We have extended the technique to the Arbitrary Lagrangian Eulerian (ALE) framework in Guermond et al. [15]. The method has been applied to the shallow water system in Guermond et al. [9] (this work was done in close collaboration with the U.S. Army Engineer Research and Development Center (ERDC)). An extension to a dispersive shallow water model supporting solitary waves has been developed in Guermond et al. [13]. As an illustration of the versatility of the technique proposed by the PIs, we show in Figure 1 a snapshot of a simulation of the flow at Mach 3 around a cylinder in a channel. These results have been obtained using a massively parallel code exactly implementing the method described in [8, 12]. This simulation have been done with 1.8 billion grid points using continuous $\mathbb{Q}_1$ finite elements. The code has been written, debugged and validated in a few months with the finite element library `deal.II` by Matthias Maier (TAMU) and Martin Kronbichler (Tech. Univ. Munich), [20]. The astonishing success of this project achieved is such a short time frame is a clear indication of the robustness, simplicity, and versatility of the proposed methodology.

Figure 1: Cylinder in a channel at Mach 3, 1.8B grid points



Compressible Navier-Stokes We have extended our invariant-domain preserving technique to the compressible Navier-Stokes equations. We present in Guermond et al. [19, 18] a fully discrete approximation technique for the compressible Navier-Stokes equations that is second-order accurate in time and space, semi-implicit, and guaranteed to be invariant domain preserving. The restriction on the time step is the standard hyperbolic CFL condition, i.e., $\tau \lesssim \mathcal{O}(h)/V$ where V is some reference velocity scale and h the typical meshsize. We illustrate the method in Figure 2. It is a snapshot of the density of the Navier-Stokes flow around the airfoil OAT15a in the transonic regime at Reynolds number Re $= 3{\times}10^6$. No turbulence modeling of any sort is used. The accuracy of the method is achieved by using highly anisotropic cells in the viscous boundary layer.

Figure 2: OAT15a foil in transonic regime, Re $= 3{\times}10^6$. Density snapshot.



Positivity and structure preservation for radiative transport: The PIs have extended the technique to the one-group radiative transport equation. This equation (akin to the Boltzmann equation) is a key step in the development of numerical methods for the so-called rad-hydro system which couples radiation and hydrodynamics. This system is important in many astrophysics, DoE, and DoD applications. We published a breakthrough paper in 2020 in this field, Guermond et al. [14]. We propose a finite element technique that preserves positivity of the solution and is asymptotic preserving in the diffusion limit. To the best of the PIs knowledge, this paper is the very first one achieving this result with finite elements. This key result is an important step towards the development of robust approximations of the full rad-hydro system.

Tabulated equations of state Real non-ideal gases are composed of molecules that occupy space and interact; consequently, they do not adhere to the ideal gas law and the ideal gas equation of state cannot be used to model such physical processes. The ideal gas equation of state cannot account for finite compressibility effects, variable specific heat capacity, van der Waals forces, and other thermodynamic effects. Many alternative models can be used in theses cases, but for the majority of these models finding the exact solution in the one-dimensional Riemann problem is either extremely complicated (Van der Waals, Redlich-Kwong, Mie-Gruneisen equations of state) or just impossible (tabulated equations of state). In all of these situations it is either very challenging or impossible to compute an upper bound on the maximum wave speed in the one-dimensional Riemann problem. Since the robustness of numerical approximations depend on this upper bound, it becomes clear that a general framework is needed to deal with real gases. We have developed such a method in B. Clayton [2]. This methods guarantees that the numerical solution is thermodynamically consistent.

2 Impacts

2.1 Collaborations, Mentoring, and Training

We describe in this section the collaborations, mentoring, training, and professional development the PIs have engaged in during the grant period.

Collaborations and mentoring. Three graduate students have been partially supported by this grant. One of them (Hua Yuchen) graduated in 2019 and now holds a tenure-track position at the Univ. of Sci. and Tech. of China, Hefei, China. Another one (Eric Tovar) is going to graduate in Fall 2021. He had three summer internships at the U.S. Army Engineer Research and Development Center, Vicksburg, MI. He transitions the techniques that we develop for the shallow water equation into ERDC's codes. The third student (Bennett Clayton) is going to graduate in 2022. He works on nonstandard and tabulated equations of states. One postdoctoral researcher (Ignacio Tomas) was partially supported by the grant. He now holds an associate researcher position at Sandia National Laboratories, Albuquerque, NM. Most of the work done with the support of the grant was done in association with DoE and DoD affiliated institutions. Great efforts are made to transition the results to these institutions, either through internships, direct collaborations, or monthly meetings. We also collaborate with the BLAST team at the Lawrence Livermore National Laboratory, Livermore. We also used the grant to support the visits of Laura Saavedra (Assist. Prof., Universidad Politécnica de Madrid) who works with us on compressible Lagrangian hydrodynamics.

Personnel Supported During Duration of Grant. The following persons have been supported or partially supported by the grant.

1. Jean-Luc Guermond, Professor, Texas A&M University.
2. Bojan Popov, Professor, Texas A&M University.
3. Eric Tovar, Graduate student, Texas A&M University (graduated in 2021).
4. Bennett Clayton, Graduate student, Texas A&M University (will graduate in 2022).

Dissemination. All the results obtained during the 2018-2021 period have been submitted to specialized scientific journals and have been presented at various conferences and workshops.

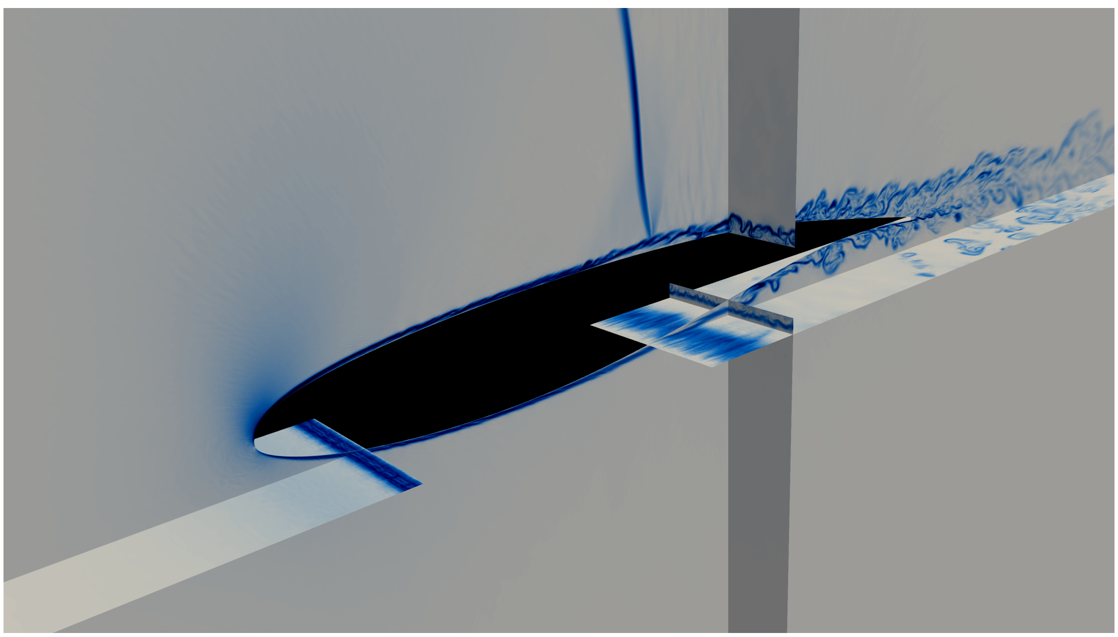
3 Changes

No changes were made.

4 Technical Updates

The invariant domain preserving technique that we developed for solving generic hyperbolic systems has been implemented in Deal.II using continuous Q1 elements in 2 and 3 dimensions. The code has been specialized for the compressible Euler and Navier-Stokes equations and the dispersive shallow water equations. The method scales extremely well on hybrid architectures. We have demonstrated that the technique has excellent weak and strong scaling using hybrid thread/MPI parallelization. Some outputs from the code are shown in Figures 3, 5, and 6.

Figure 3: Airfoil OAT15a at Re=3 000 000, 3D, schlieren plot of density



References

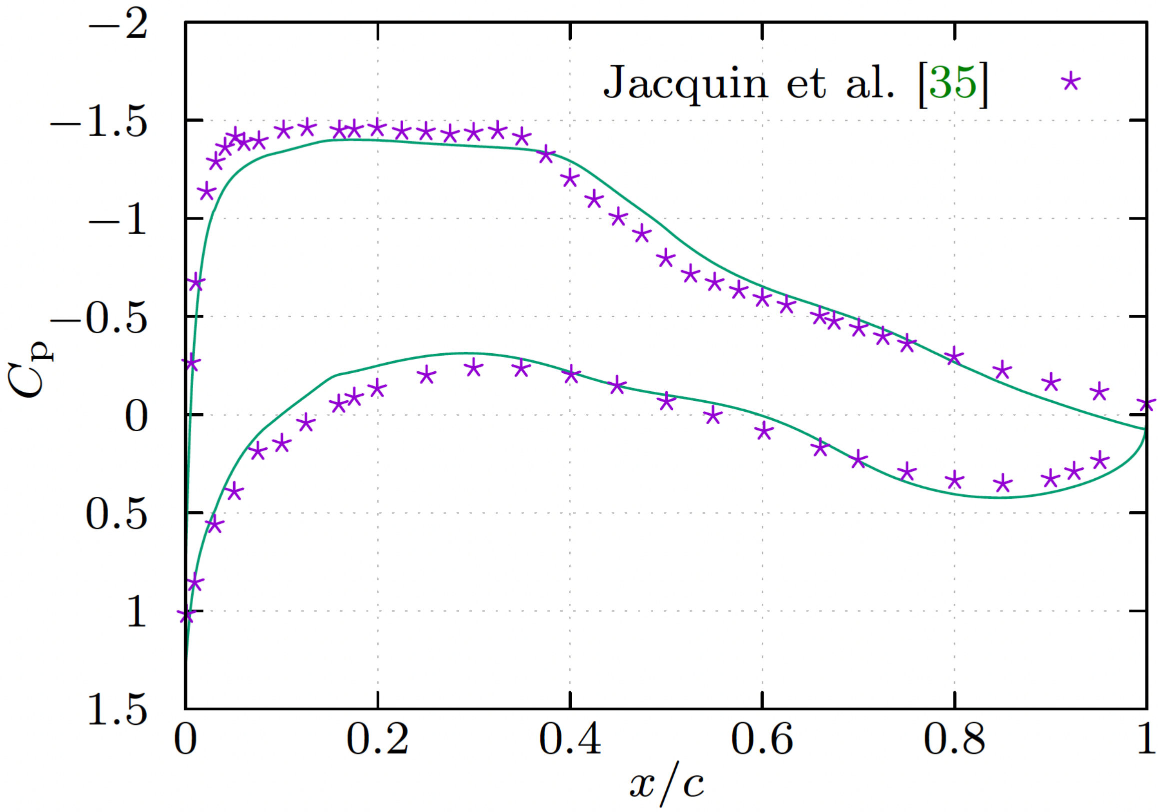
[1] P. Azerad, J.-L. Guermond, and B. Popov. Well-balanced second-order approximation of the shallow water equation with continuous finite elements. *SIAM J. Numer. Anal.*, 55(6):3203–3224, 2017.

[2] B. P. B. Clayton, J.-L. Guermond. Invariant-domain preserving approximations for the euler equations with tabulated equation of state. *SIAM J. Sci. Comput.*, 2021. In review.

[3] J.-L. Guermond and B. Popov. Invariant domains and first-order continuous finite element approximation for hyperbolic systems. *SIAM J. Numer. Anal.*, 54(4):2466–2489, 2016.

[4] J.-L. Guermond and B. Popov. Invariant domains and second-order continuous finite element approximation for scalar conservation equations. *SIAM J. Numer. Anal.*, 55(6):3120–3146, 2017.

Figure 4: Airfoil OAT15a at Re=3 000 000, 3D. Time average and spanwise average of the pressure coefficient on the pressure side and the suction side of the foil. Comparison betweeen experiments and our computations



[5] J.-L. Guermond, M. Q. de Luna, and T. Thompson. An conservative anti-diffusion technique for the level set method. *J. Comput. Appl. Math.*, 321:448–468, 2017.

[6] J.-L. Guermond, B. Popov, L. Saavedra, and Y. Yang. Invariant domains preserving arbitrary Lagrangian Eulerian approximation of hyperbolic systems with continuous finite elements. *SIAM J. Sci. Comput.*, 39(2):A385–A414, 2017.

[7] J.-L. Guermond, B. Popov, and Y. Yang. The effect of the consistent mass matrix on the maximum-principle for scalar conservation equations. *J. Sci. Comput.*, 70(3):1358–1366, 2017.

[8] J.-L. Guermond, M. Nazarov, B. Popov, and I. Tomas. Second-order invariant domain preserving approximation of the Euler equations using convex limiting. *SIAM J. Sci. Comput.*, 40(5):A3211–A3239, 2018.

[9] J.-L. Guermond, M. Quezada de Luna, B. Popov, C. E. Kees, and M. W. Farthing. Well-balanced second-order finite element approximation of the shallow water equations with friction. *SIAM J. Sci. Comput.*, 40(6):A3873–A3901, 2018.

[10] J.-L. Guermond, C. Klingenberg, B. Popov, and I. Tomas. The Suliciu approximate Riemann solver is not invariant domain preserving. *J. Hyperbolic Differ. Equ.*, 16(1):59–72, 2019.

[11] J.-L. Guermond, B. Popov, L. Saavedra, and Y. Yang. Arbitrary Lagrangian-Eulerian finite element method preserving convex invariants of hyperbolic systems. In *Contributions to partial differential equations and applications*, volume 47 of *Comput. Methods Appl. Sci.*, pages 251–

Figure 5: Scaling analysis of the 3D Onera OAT15a airfoil on up to 2,048 nodes (i.e., 98,304 cores) of SuperMUC-NG. In the left panel, the strong and weak scaling of five different problem sizes is assessed, involving up to 17.4 billion grid points (Qdofs) (i.e., 85 billion unknowns). In the right panel, the time per time step for the case with 34.5 million grid points is broken down to show the contributions of the hyperbolic and parabolic parts.

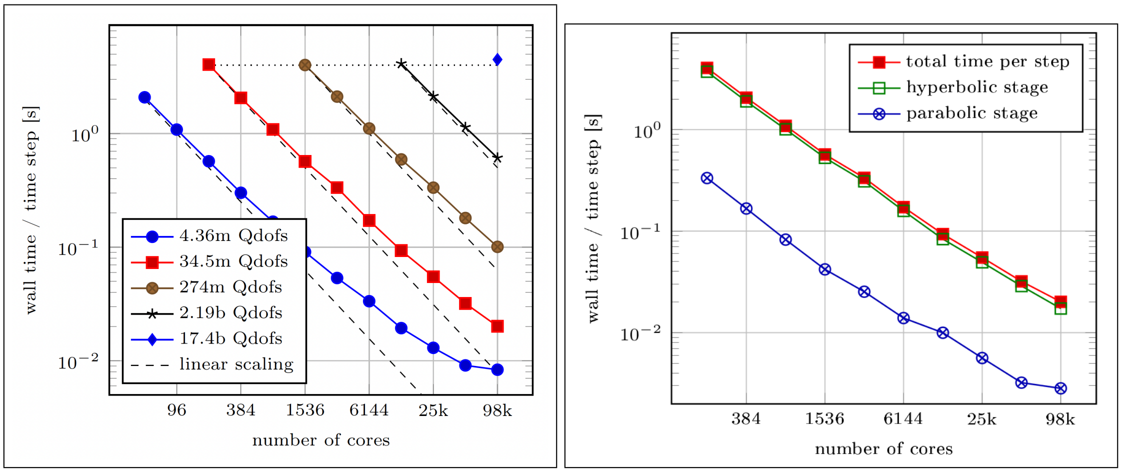
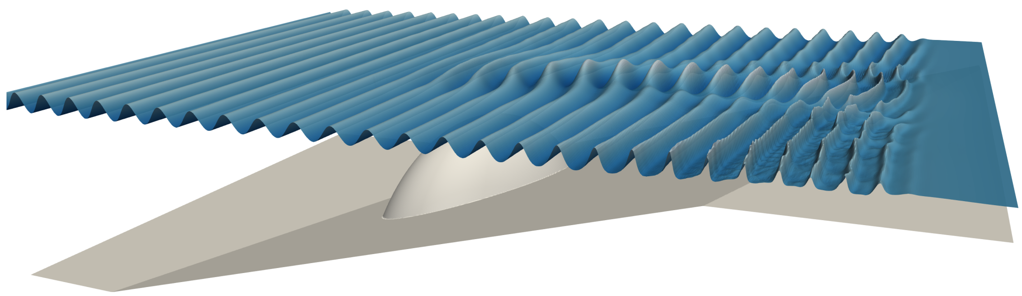


Figure 6: Periodic wave shoaling over an immersed reef using the Serre–Green-Nagdhi equations



272. Springer, Cham, 2019.

[12] J.-L. Guermond, B. Popov, and I. Tomas. Invariant domain preserving discretization-independent schemes and convex limiting for hyperbolic systems. *Comput. Methods Appl. Mech. Engrg.*, 347: 143–175, 2019.

[13] J.-L. Guermond, B. Popov, E. Tovar, and C. Kees. Robust explicit relaxation technique for solving the Green-Naghdi equations. *J. Comput. Phys.*, 399:108917, 17, 2019.

[14] J.-L. Guermond, B. Popov, and J. Ragusa. Positive and asymptotic preserving approximation of the radiation transport equation. *SIAM J. Numer. Anal.*, 58(1):519–540, 2020.

[15] J.-L. Guermond, B. Popov, and L. Saavedra. Second-order invariant domain preserving ALE approximation of hyperbolic systems. *J. Comput. Phys.*, 401:108927, 26, 2020.

[16] J.-L. Guermond, C. Kees, B. Popov, and E. Tovar. Hyperbolic relaxation technique for solving the dispersive serre–green–naghdi equations with topography. *J. Comput. Phys.*, 2021. Under review.

[17] J.-L. Guermond, C. Kees, B. Popov, and E. Tovar. Well-balanced second-order convex limiting technique for solving the serre equations. *Water waves*, 2021. Under review.

[18] J.-L. Guermond, M. Kronbichler, M. Maier, B. Popov, and I. Tomas. On the implementation of a robust and efficient finite element-based parallel solver for the compressible navier–stokes

equations. *Comput. Methods Appl. Mech. Engrg.*, 2021. in press.

[19] J.-L. Guermond, M. Maier, B. Popov, and I. Tomas. Second-order invariant domain preserving approximation of the compressible Navier-Stokes equations. *Comput. Methods Appl. Mech. Engrg.*, 375:113608, 17, 2021.

[20] M. Maier and M. Kronbichler. Efficient parallel 3D computation of the compressible Euler equations with an invariant-domain preserving second-order finite-element scheme. *ACM Transactions on Parallel Computing*, 8(2):in press, 2021.

[21] B. Popov and Y. Hua. Invariant domain preserving central schemes for nonlinear hyperbolic systems. *Comm. Math. Sci.*, 2021.