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Variational–Sturm–Liouville Modeling of Structured Transport

The Mathematical Foundation of the AstraNomos PRISM Simulation Engine

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ABSTRACT

Modern simulation tools for heat transfer, turbulence, and complex transport systems typically rely on diffusion-based models derived from Fourier’s law or stochastic approximations of the Navier–Stokes equations. While these approaches are highly successful in regimes where transport is smooth and weakly structured, they often fail to capture localized energy amplification, confinement effects, and structured transport pathways observed in real systems.

This paper introduces the mathematical foundation underlying the AstraNomos PRISM Simulation Engine: a unified variational formulation of transport governed by a self-adjoint Sturm–Liouville operator with curvature potential. Starting from a Euler–Lagrange functional, we derive a transport equation in which entropy-dependent mobility and curvature energy determine the admissible evolution of the system. The resulting operator possesses a well-defined spectral structure whose eigenfunctions represent the natural transport modes of the medium.

Within this framework, classical Fourier diffusion emerges as a special limiting case when curvature energy vanishes. When geometric confinement becomes active, however, the operator spectrum localizes, producing persistent hotspots, channelized transport, and structured energy flow patterns. This mathematical structure provides the core theoretical basis for the PRISM simulation engine, enabling digital twins to detect hidden transport structure that conventional models treat as stochastic noise.

From a computational standpoint, traditional simulation workflows—particularly in computational fluid dynamics (CFD) and thermal transport modeling—require resolving governing equations across extremely large spatial discretizations. Engineers typically construct high-resolution meshes containing millions or billions of degrees of freedom and solve the governing equations iteratively across time or pseudo-time. Because localized transport structures such as vortices, recirculation zones, or thermal hotspots emerge only after many nonlinear solver iterations, these models often require substantial computational resources, long simulation times, and extensive turbulence closure schemes to approximate unresolved dynamics.

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The structured operator formulation underlying the PRISM Simulation Engine alters this computational paradigm by shifting the focus from brute-force discretization to the spectral structure of the governing transport operator. Instead of resolving the full field through dense spatial meshes, the transport dynamics are projected onto the eigen-basis of the self-adjoint Sturm–Liouville operator governing the system. In practical terms, this means that the dominant transport behavior of a system can often be represented by a relatively small number of operator modes that capture the admissible energy pathways of the geometry.

This spectral representation dramatically reduces the dimensionality of the computational problem. Whereas classical CFD models must solve large coupled systems of algebraic equations corresponding to every mesh element, the PRISM framework evolves the system within a reduced modal space determined by the operator spectrum. When the transport physics is governed by a small number of dominant modes—as is frequently the case in confinement-dominated regimes—the resulting computational problem becomes orders of magnitude smaller while still capturing the essential physics of the system.

Another advantage of the structured operator framework is that it naturally separates diffusion-dominated regimes from confinement-dominated regimes. In traditional simulation pipelines, these regimes must be discovered indirectly through mesh refinement or turbulence modeling. In the PRISM framework, the spectral properties of the operator immediately indicate whether transport is governed by diffuse smoothing or by localized confinement modes. This allows simulations to allocate computational effort only where structured transport occurs, rather than uniformly across the entire domain.

As a result, the PRISM approach provides not only a more physically interpretable model of transport dynamics but also a more computationally efficient simulation strategy. By identifying the natural transport modes of the system directly from the governing operator, the framework avoids the need for excessive numerical resolution while still capturing localized amplification phenomena. For engineers working with complex thermal, fluid, or energy systems, this approach enables faster simulation cycles, reduced computational cost, and earlier identification of critical transport structures that would otherwise remain hidden within conventional diffusion-based models.

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Simulation technology plays a central role in modern engineering and scientific analysis. From reactor cooling networks and turbine blades to semiconductor thermal management and plasma systems, predictive models allow engineers to analyze complex physical processes before systems are built or failures occur. Most contemporary simulation frameworks ultimately rely on diffusion-based transport models. Fourier heat conduction provides the canonical description:

$$\frac{\partial u}{\partial t} = \kappa \Delta u$$

where u represents temperature or energy density and κ is the diffusivity constant. This formulation assumes that energy spreads smoothly across a domain, producing progressively uniform distributions over time. While this assumption works well in many situations, it fails in systems where geometry, confinement, or structural heterogeneity strongly influence transport.

In such environments, energy does not spread uniformly. Instead, it forms localized structures such as:

- Thermal hotspots in turbine blades
- Channelized flow in packed-bed reactors
- Localized plasma transport pathways
- Persistent heat concentrations in electronic systems.

Traditional diffusion models often interpret these structures as stochastic fluctuations or turbulence-driven irregularities. However, a growing body of evidence suggests that these phenomena reflect deeper geometric structure in the governing transport dynamics. The AstraNomos research program approaches this problem from a different perspective: instead of treating transport as purely diffusive, it models transport through a structured operator framework derived from variational principles.

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2. Variational Formulation of Structured Transport

Consider a bounded domain:

$$\Omega \subset \mathbb{R}^n$$

with smooth boundary $\partial\Omega$.

Let

- $S(x)$ denote the structured entropy scalar field,
- $D(S)$ denote entropy-dependent mobility,
- $V(x)$ denote curvature potential energy.

We begin by defining a quadratic functional representing total transport energy:

$$J[u] = \int_{\Omega} (D(S) |\nabla u|^2 + V(x)u^2) dx - \int_{\Omega} fu dx$$

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The functional contains two primary energy contributions:

1. **Transport energy**

$$D(S) |\nabla u|^2$$

representing admissible smoothing dynamics.

2. **Curvature potential energy**

$$V(x)u^2$$

representing confinement induced by geometric structure. Stationary points of the functional correspond to physically admissible transport states.

Taking the first variation:

$$\delta J = 0$$

and applying integration by parts yields the Euler–Lagrange equation:

$$-\nabla \cdot (D(S)\nabla u) + V(x)u = f.$$

This equation defines the fundamental operator governing structured transport.

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3. The Unified Transport Operator

The governing operator may be written compactly as:

$$\mathcal{L}u = -\nabla \cdot (D(S)\nabla u) + V(x)u.$$

This operator possesses several important properties:

Self-adjointness

Under the inner product:

$$\langle u, v \rangle = \int_{\Omega} uv \, dx$$

the operator satisfies:

$$\langle \mathcal{L}u, v \rangle = \langle u, \mathcal{L}v \rangle.$$

Thus, the operator is symmetric.

Ellipticity

If

$$D(S) \geq c_0 > 0$$

then the operator is uniformly elliptic.

Coercivity

Since $V(x) \geq 0$, the associated bilinear form:

$$a(u, u) = \int_{\Omega} (D(S) |\nabla u|^2 + V(x)u^2) dx$$

is coercive. By the Lax–Milgram theorem and Friedrichs extension, the operator admits a unique self-adjoint realization on the Hilbert space $L^2(\Omega)$.

4. Sturm–Liouville Structure

In one dimension the operator reduces to canonical Sturm–Liouville form:

$$-(p(x)u')' + q(x)u = f(x)$$

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where:

$$p(x) = D(S), q(x) = V(x).$$

The associated eigenvalue problem:

$$\mathcal{L}\phi_k = \lambda_k \phi_k$$

generates a discrete spectrum:

$$0 < \lambda_1 \leq \lambda_2 \leq \dots .$$

The eigenfunctions form an orthogonal basis of the solution space. Thus, any transport field can be expressed as:

$$u(x) = \sum_{k=1}^{\infty} c_k \phi_k(x).$$

Within this framework, transport is governed by the spectral structure of the operator rather than purely by diffusion.

5. Spectral Transport Modes

The eigenfunctions of the operator represent natural transport modes of the medium. Two regimes emerge depending on the relative strength of the curvature potential.

Diffusion-dominated regime

If

$$V(x) \approx 0$$

then the operator reduces to:

$$\mathcal{L} \approx -D\Delta.$$

The spectrum resembles that of the Laplacian, and eigenfunctions remain delocalized. Energy spreads smoothly across the domain, consistent with classical diffusion.

Confinement-dominated regime

When curvature potential becomes significant,

$$V(x) \gg D(S) |\nabla^2|.$$

Low-lying eigenfunctions localize around minima of $V(x)$.

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These localized modes correspond to:

- Persistent hotspots
- Channelized transport
- Confined energy pathways.

This phenomenon explains many transport structures observed in real systems.

6. Classical Limit: Recovery of Fourier Diffusion

An important property of the unified operator is that it reduces exactly to classical diffusion when curvature vanishes. If:

$$V(x) = 0$$

and

$$D(S) = D_0$$

then

$$\mathcal{L}u = -D_0\Delta u.$$

Thus, the classical Fourier heat equation is recovered without approximation. This result demonstrates that the structured operator framework is not a replacement for diffusion models but a generalization of them.

7. Confinement Parameter

To characterize regime transitions we define a nondimensional confinement parameter:

$$\theta = \frac{\int_{\Omega} V(x) u^2 dx}{\int_{\Omega} D(S) |\nabla u|^2 dx}$$

This ratio measures the relative strength of curvature confinement to diffusion smoothing. Two regimes follow:

$$\begin{aligned} \theta \ll 1 &\Rightarrow \text{diffusion dominated} \\ \theta \gg 1 &\Rightarrow \text{confinement dominated.} \end{aligned}$$

In the confinement regime, eigenfunctions localize near curvature wells, producing persistent transport structures.

8. Implications for Simulation Technology

The mathematical framework described above forms the theoretical basis for the AstraNomos PRISM Simulation Engine. Instead of modeling transport purely through diffusion equations, PRISM analyzes the spectral structure of the governing operator. This enables the engine to detect transport modes that conventional models smooth away.

In practical simulations this allows PRISM to identify:

- Hidden thermal pathways in turbine blades
- Cooling instabilities in reactor systems
- Transport channels in packed-bed reactors
- Structured heat flow in semiconductor arrays.

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In each case, the engine computes the spectral response of the operator to system forcing, revealing the true transport modes of the system.

To understand how this enhances simulation technology, consider how a typical engineering transport simulation is performed using conventional computational fluid dynamics (CFD). Suppose an engineer wishes to simulate heat transport in a reactor cooling channel or data-center airflow system. The governing equation typically takes the form:

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p (\mathbf{u} \cdot \nabla T) = \nabla \cdot (k \nabla T) + Q$$

where T is temperature, \mathbf{u} is the velocity field, k is thermal conductivity, and Q is a source term. To solve this equation numerically, the spatial domain must be discretized into a mesh of M grid cells. The resulting discretized system becomes a large coupled algebraic system of the form:

$$A\mathbf{T} = \mathbf{b}$$

where A is an $M \times M$ matrix representing diffusion and convection operators and \mathbf{T} is the vector of nodal temperatures. In realistic industrial problems, M may range from 10^6 to 10^9 unknowns. Solving such systems requires iterative solvers and turbulence closures, and the computational complexity typically scales roughly as:

$$\mathcal{O}(M \cdot N_{\text{iter}})$$

where N_{iter} is the number of solver iterations. When localized flow structures or thermal hotspots appear, additional mesh refinement is often required, further increasing the computational burden. The PRISM framework approaches the problem differently by exploiting the spectral structure of the governing transport operator:

$$\mathcal{L}u = -\nabla \cdot (D(S)\nabla u) + V(x)u.$$

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Instead of solving directly for the full spatial field at every grid point, the solution is expanded in the eigenbasis of this operator:

$$u(x, t) = \sum_{k=1}^N a_k(t) \phi_k(x),$$

where $\phi_k(x)$ are the eigenfunctions of \mathcal{L} and $a_k(t)$ are the modal amplitudes. The key observation is that the dominant transport physics of many systems is captured by a relatively small number of eigenmodes N , where typically:

$$N \ll M.$$

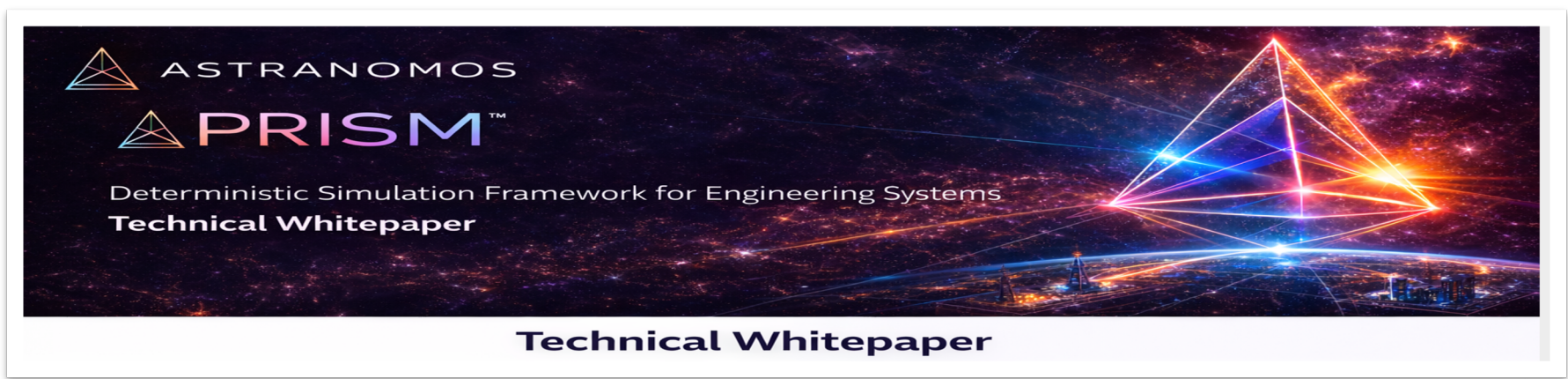
The governing dynamics therefore reduce to a lower-dimensional system for the modal coefficients:

$$\frac{da_k}{dt} + \lambda_k a_k = f_k,$$

where λ_k are the eigenvalues of the operator and f_k are projections of the forcing terms. Instead of evolving millions of spatial variables, the simulation evolves only the modal amplitudes associated with the physically admissible transport modes.

To illustrate the dimensionality reduction, consider a simplified industrial example. A CFD simulation of a cooling system might involve $M = 10^7$ mesh nodes. A traditional solver must compute the temperature field at all nodes for each iteration. In contrast, if the dominant transport behavior is governed by approximately $N = 100$ operator modes, the PRISM framework evolves only those 100 modal amplitudes. The computational complexity therefore reduces from:

$$\mathcal{O}(10^7)$$



degrees of freedom to:

$$\mathcal{O}(10^2)$$

modal coefficients governing the dominant physics. Even when the eigen-basis must initially be computed, the resulting reduced-order representation can accelerate repeated simulations dramatically.

Another advantage of this formulation is that the spectral operator immediately reveals whether a system lies in a diffusion-dominated or confinement-dominated regime. In classical CFD workflows this distinction must be inferred through turbulence models or mesh refinement. In the structured operator framework, it emerges directly from the relative strength of the curvature potential $V(x)$. When confinement dominates, the operator eigenfunctions localize around geometric wells, indicating the presence of hotspots or structured transport channels. Engineers can therefore identify these regions without resolving the entire domain at extremely high resolution.

From a computational standpoint, the key advantage of the structured operator framework is that it reduces the effective degrees of freedom required to represent the physical system. In conventional CFD workflows, the governing equations are discretized across a spatial mesh with M nodes, meaning that the solver must evolve M unknown variables. For realistic industrial simulations, this may involve millions or billions of degrees of freedom. However, most of these variables exist only because the solver is attempting to reconstruct transport structure indirectly through brute-force discretization.

The PRISM framework instead identifies the natural spectral basis of the transport operator, allowing the solution field to be expressed as:

$$u(x, t) = \sum_{k=1}^N a_k(t) \phi_k(x),$$

where $\phi_k(x)$ are eigenfunctions of the operator:

$$\mathcal{L} = -\nabla \cdot (D(S)\nabla) + V(x).$$

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9. From Mathematical Theory to Digital Twins

Within the PRISM engine, the structured operator is implemented numerically through discretization of the governing functional. The resulting digital twin solves the resolvent equation:

$$(\mathcal{L}-\lambda I)^{-1}f$$

under system forcing.

The computed spectral response reveals:

- Dominant transport modes
- Localization regions
- Potential hotspot zones.

Because the operator remains self-adjoint, the simulation retains strong stability and interpretability properties.

10. Conclusion

This paper has presented the mathematical framework underlying the AstraNomos PRISM Simulation Engine. Starting from a variational principle, we derived a self-adjoint transport operator combining entropy-dependent mobility with curvature confinement potential. The resulting equation forms a Sturm–Liouville system whose spectral structure governs admissible transport modes in complex media. Several key conclusions follow.

First, classical Fourier diffusion emerges as a limiting case of the unified operator. When curvature potential and entropy structure vanish, the governing equation reduces exactly to the classical heat operator. In this sense, the structured formulation does not replace traditional diffusion models but extends them into regimes where geometry and confinement become dynamically relevant.

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Second, curvature potentials produce localized transport modes corresponding to hotspots, channelized transport, and persistent energy structures. These phenomena frequently appear in practical systems—such as turbine blades, packed-bed reactors, reactor cooling networks, and semiconductor thermal fields—where traditional diffusion models tend to smooth away physically meaningful structure.

Third, the spectral basis of the operator provides a natural representation of admissible motion in structured media. Instead of interpreting complex transport patterns as stochastic irregularities, the structured formulation identifies them as projections onto the eigenmodes of the governing operator.

To understand the practical significance of this result, it is useful to compare the structured operator framework with traditional simulation pipelines. Classical engineering simulation typically begins with governing equations such as the Navier–Stokes equations or Fourier heat transport, followed by numerical discretization and turbulence or closure models. Because many of these models assume smooth diffusion behavior, the resulting simulations often average away localized transport pathways that emerge from geometry and confinement.

The PRISM framework enhances this workflow by introducing an operator-based spectral layer above the classical transport equations. Rather than altering the underlying physics, the framework analyzes the structure of the governing operator itself, identifying when transport dynamics depart from pure diffusion and enter confinement-dominated regimes. In practice, this allows simulations to detect when hotspots, channelized flows, or localized transport modes will emerge before they become visible in coarse diffusion fields.

From an engineering perspective, this layered approach allows traditional simulation tools to remain useful while augmenting them with deeper diagnostic capability. Diffusion models remain accurate in weakly structured regimes, but when curvature or confinement activates, the spectral structure of the operator reveals the underlying transport pathways governing the system. In this sense, the PRISM framework functions as a structured diagnostic engine embedded within the broader simulation workflow.

These results form the theoretical backbone of the AstraNomos PRISM Simulation Engine and establish a pathway toward a new generation of physics-driven digital twins capable of interpreting complex physical systems with greater fidelity. By combining classical transport theory with spectral operator analysis, the framework provides a unified approach to simulation in which diffusion, confinement, and structured transport all emerge naturally from the same mathematical foundation.

Building on this foundation, the structured operator framework also offers a new perspective on how complex simulations are performed in computational fluid dynamics (CFD) and related numerical modeling fields. Traditional CFD workflows typically rely on solving large systems of nonlinear

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partial differential equations—often the Navier–Stokes equations—through fine spatial discretization and iterative time stepping. While this approach is highly accurate, it can be computationally intensive, requiring extremely high mesh resolution and turbulence modeling schemes to capture localized phenomena such as vortices, recirculation zones, or thermal amplification regions. In many cases, the computational burden arises from the need to resolve these structures indirectly through brute-force numerical refinement.

The PRISM operator framework introduces an alternative layer of analysis by focusing directly on the spectral structure of the governing transport operator. Instead of resolving every small-scale feature through increasingly dense meshes, the method identifies the dominant eigenmodes that govern transport behavior in the system. Because these eigenmodes correspond to the natural transport pathways of the geometry, they allow simulations to capture the essential dynamics of the system with significantly reduced numerical overhead. In effect, the operator-based approach identifies the meaningful degrees of freedom in the system rather than attempting to resolve every possible fluctuation.

This spectral perspective can dramatically reduce the amount of computational “heavy lifting” required in many simulation tasks. When the dominant transport modes of a system are known, simulations can be projected onto a reduced spectral basis that captures the most relevant energy pathways. Instead of solving for millions of mesh elements across a full domain, the simulation can evolve along a smaller set of operator modes that represent the physically admissible transport structures. This approach is conceptually similar to reduced-order modeling but is grounded directly in the physics of the governing operator rather than in purely empirical dimensionality reduction.

Beyond CFD, the same principle applies to other domains where simulation complexity grows rapidly with system size. Thermal transport modeling, reactor cooling analysis, plasma transport simulations, and large-scale energy systems often rely on high-resolution numerical solvers to approximate the behavior of complex physical fields. By incorporating the structured operator framework, these simulations can identify confinement regimes and transport channels early in the modeling process, allowing computational resources to focus on the regions where structure actually emerges rather than expending equal effort across the entire domain.

From a practical engineering standpoint, this shift represents a refinement in how simulations are interpreted and executed. Instead of treating complexity as an obstacle that must be overcome through brute computational force, the PRISM framework treats complexity as a manifestation of underlying operator structure. By identifying and exploiting that structure, simulations can become both faster and more physically interpretable, enabling engineers to move more efficiently from raw numerical models to actionable insights about system behavior.

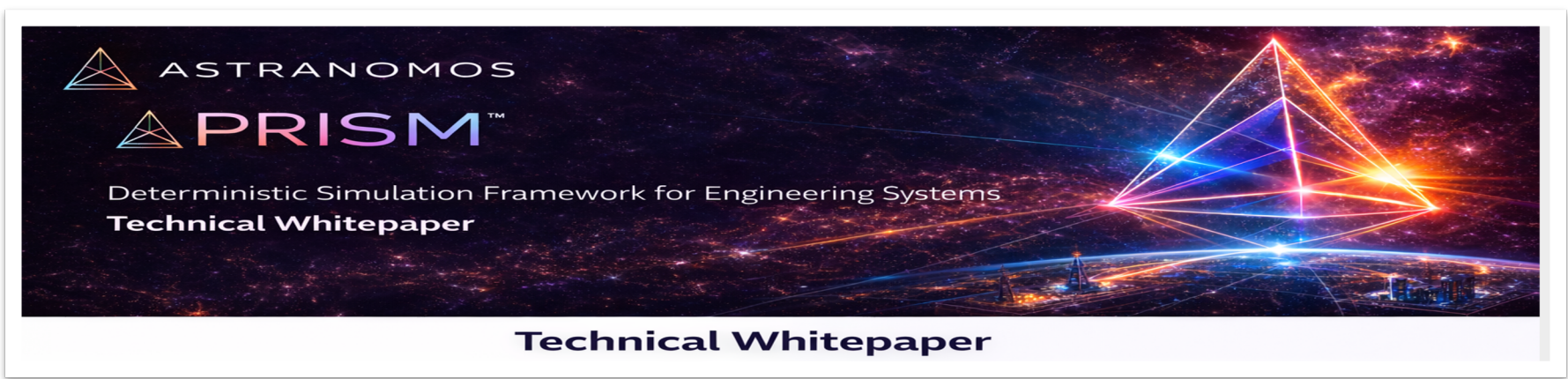
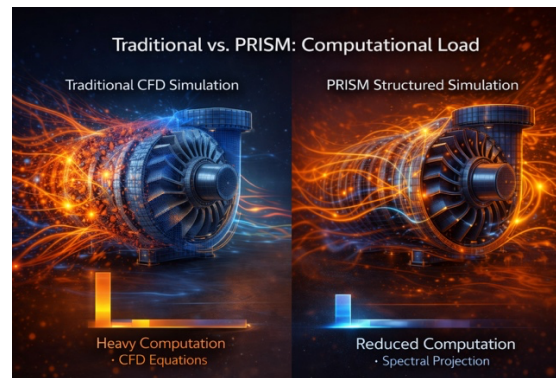


Figure 1.



Engineers performing simulation today typically approach complex transport problems through statistical or turbulence-closure methods layered on top of numerical discretizations of governing equations. Consider a typical CFD thermal analysis of a data-center rack. The engineer begins with the heat transport equation coupled to Navier–Stokes flow:

$$\rho c_p \frac{\partial T}{\partial t} + \rho c_p (\mathbf{u} \cdot \nabla T) = \nabla \cdot (k \nabla T) + Q$$

Because the velocity field \mathbf{u} and turbulent transport terms cannot be resolved exactly at practical grid resolutions, engineers introduce statistical turbulence closures, such as k - ϵ or Reynolds-averaged models. In practice, this means solving for ensemble-averaged quantities:

$$u_i \bar{u}_j = R_{ij}$$

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and approximating transport through effective diffusivity terms:

$$k_{eff} = k + k_t$$

where k_t is a turbulence-induced diffusivity. The simulation therefore attempts to capture the true physics indirectly through mesh refinement and statistical approximations. For a large industrial model—such as a cooling system or reactor—this often requires millions to billions of grid cells and many iterative solver passes, because the solver must numerically reconstruct localized flow structures through brute-force computation.

The PRISM structured operator framework approaches the problem from a fundamentally different computational perspective. Rather than resolving the full field through dense discretization and statistical closures, the system is projected onto the spectral basis of the governing transport operator:

$$\mathcal{L}u = -\nabla \cdot (D(S)\nabla u) + V(x)u$$

where $D(S)$ represents entropy-dependent mobility and $V(x)$ is the curvature confinement potential. Instead of computing the full solution field at every grid point, the system is expanded in eigenmodes of this operator:

$$u(x, t) = \sum_{k=1}^N a_k(t)\phi_k(x)$$

where ϕ_k are the eigenfunctions of \mathcal{L} . In practical engineering simulations, the dominant transport behavior is typically captured by a relatively small number of modes $N \ll M$, where M is the number of mesh nodes required in a traditional CFD discretization. This converts the computational problem from solving a very large spatial system into evolving a reduced spectral dynamical system.

To illustrate the difference numerically, consider a typical industrial CFD problem involving 10^7 grid cells with a nonlinear solver requiring 10^3 time-steps. The effective computational workload scales roughly as

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$$\mathcal{O}(M \times N_{iter})$$

which in this case approaches 10^{10} operations per simulation cycle. In the PRISM formulation, if the dominant physics is captured by the first 50–200 eigenmodes of the operator, the system reduces to solving a spectral evolution equation for the modal coefficients $a_k(t)$:

$$\frac{da_k}{dt} + \lambda_k a_k = f_k$$

where λ_k are operator eigenvalues and f_k are projections of the forcing field. The effective computational complexity then scales as:

$$\mathcal{O}(N_{modes}^2)$$

which can be orders of magnitude smaller than the full discretized problem. In practical engineering workflows this means that simulations that previously required large HPC clusters and hours of runtime can often be reduced to far smaller spectral systems that capture the governing transport structure directly.

The visual comparison shown in the image reflects this computational shift. Traditional simulations attempt to discover transport structure indirectly through heavy numerical resolution, while the PRISM approach identifies the natural transport modes of the system first and evolves the dynamics within that structured basis. For engineers, this means fewer mesh refinements, reduced solver iteration counts, and faster convergence toward physically meaningful transport patterns. Instead of treating localized transport phenomena as statistical noise requiring additional computation, the structured operator framework interprets them as deterministic spectral modes of the system, dramatically reducing the computational effort required to simulate complex physical environments.

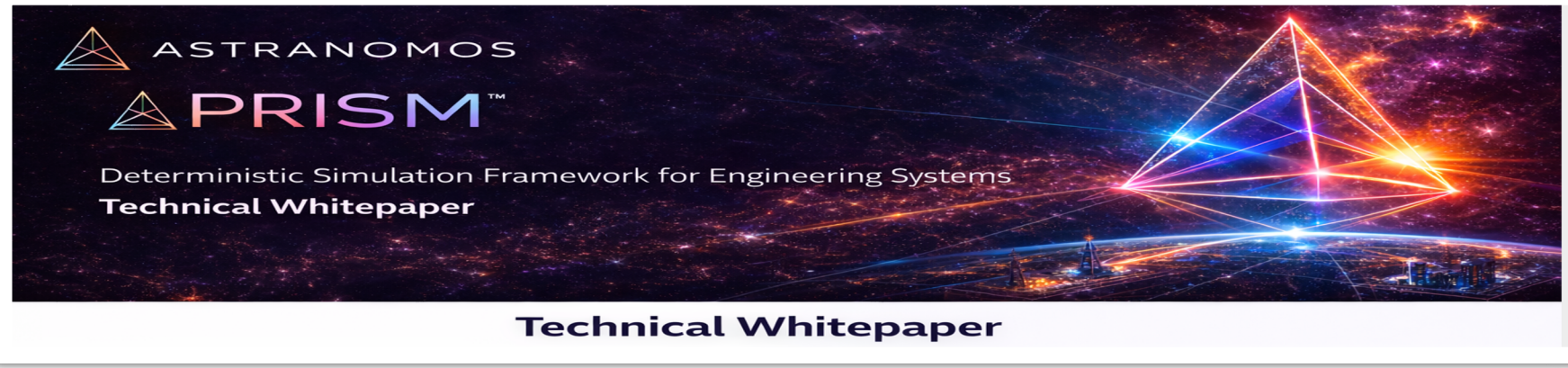
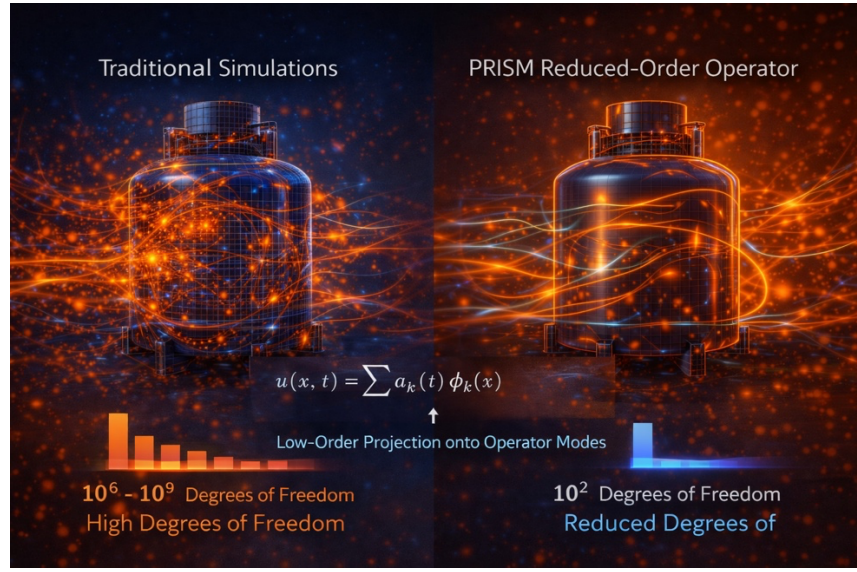


Figure 2.



The PRISM operator framework introduces determinism into the simulation by explicitly defining the admissible transport dynamics through the spectral structure of the governing operator. Rather than relying on statistical closures or turbulence models to approximate unresolved behavior, the system evolution is expressed as a projection onto the eigenmodes of the operator:

$$u(x, t) = \sum_{k=1}^N a_k(t) \phi_k(x),$$

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where the eigenfunctions $\phi_k(x)$ represent the physically admissible transport pathways of the system. Because these modes arise directly from the self-adjoint transport operator:

$$\mathcal{L}u = -\nabla \cdot (D(S)\nabla u) + V(x)u,$$

the resulting evolution of the modal amplitudes $a_k(t)$ is governed by deterministic spectral dynamics rather than by stochastic approximations. In practical engineering simulations, this means that transport phenomena traditionally treated as random fluctuations—such as localized hotspots, recirculation zones, or channelized flow—are instead interpreted as structured excitations of specific operator modes. By solving the reduced spectral system:

$$\frac{da_k}{dt} + \lambda_k a_k = f_k,$$

the PRISM engine evolves the system along the true transport basis of the geometry. The apparent randomness observed in traditional simulations therefore emerges as unresolved structure in the operator spectrum, and once the appropriate operator is defined, the dominant dynamics become predictable and reproducible. In this way, determinism is not imposed artificially on the simulation but arises naturally from the spectral closure of the governing operator. The system dynamics are confined to a well-defined set of admissible modes, allowing the simulation to capture the essential physics with far fewer degrees of freedom while maintaining a deterministic representation of the underlying transport processes.

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