Hypocoercivity-preserving Galerkin discretisations

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Canonical Example: inhomogeneous kinetic Fokker-Planck

Let $f : (0, t_f] \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, $d \in \mathbb{N}$, solution to

$$f_t + v \cdot \nabla_x f - \nabla V(x) \cdot \nabla_v f = \nabla_v \cdot (\nabla_v f + vf)$$

with ∇_x and ∇_v gradients w.r.t. x and v, respectively, subject to

$$f(0, v, x) = f_0(v, x), \qquad (v, x) \in \mathbb{R}^d \times \mathbb{R}^d,$$

for some potential $V : \mathbb{R}^d \to \mathbb{R}$ with $\int \mathrm{e}^{-V} \, \mathrm{d}x = 1$.

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The standard substitution $f = u\mathrm{e}^{-E}$, with $E(v, x) := V(x) + \frac{1}{2}|v|^2$, gives

$$u_t + v \cdot \nabla_x u - \nabla V \cdot \nabla_v u = \Delta_v u - v \cdot \nabla_v u,$$

subject to the initial condition with $u_0 := f_0 \mathrm{e}^E$.

Decay to equilibrium?

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Key property

The solution u decays to the equilibrium distribution exponentially in time.

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Energy argument: test with $u\mathrm{e}^{-E}$ and integrate w.r.t. v, x to get

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u\|^2_{L_2(\mu)} + \|\nabla_v u\|^2_{L_2(\mu)} = 0,$$

since $(v \cdot \nabla_x u - \nabla V \cdot \nabla_v u, u)_{L_2(\mu)} = 0.$

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If spectral gap/Poincaré-type inequality of the form

$$\|u - \int u \,\mathrm{d}\mu\|_{L_2(\mu)}^2 \leq \frac{2}{\kappa}\|\nabla_v u\|_{L_2(\mu)}^2 \qquad (*)$$

holds (see, e.g., Bakry & Emery ('86)),

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holds (see, e.g., Bakry & Emery ('86)), then Grönwall's Lemma gives

$$\|u(t_f) - \bar{u}\|^2_{L_2(\mu)} \le \mathrm{e}^{-\kappa t_f}\|u_0 - \bar{u}\|^2_{L_2(\mu)}$$

i.e., exponential decay to the equilibrium state $\bar{u}$ as $t_f \to \infty$.

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Key challenge

$(*)$ does *not* hold due to x dependence of μ: non-trivial kernel...

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PDE problem, together with suitable conditions:

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Let $e = u - u_h$ the error; then

$$\partial e + \mathfrak{L}_h e = \partial u - u_t + (\mathfrak{L}_h - \mathfrak{L})u + f - f_h$$

If no Poincaré inequality of the form $(\mathfrak{L}_h u, u) \gtrsim \|u\|^2$ holds.... $\rightsquigarrow$ error bound constants grow to infinity as $t \to \infty$...

Hypocoercivity (Hérau, Nier ('04), Villani ('09))

$$u_t + \mathfrak{L}u = 0 \qquad \text{where} \qquad \mathfrak{L} := \sum_{j=1}^{r} X_j^* X_j + X_0$$

with X_j 1st order diff. operators and X_0 skew-symmetric, i.e., $(X_0 v, v) = 0$.

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for some well chosen $\alpha, \beta, \gamma > 0$, which can give potentially rise to spectral gap:

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therefore, decay as $t \to \infty$: $\quad \|\mathrm{e}^{-\mathfrak{L} t}\|_{\mathcal{H}^1/\mathrm{Ker}\,\mathfrak{L} \to \mathcal{H}^1/\mathrm{Ker}\,\mathfrak{L}} \leq \mathrm{e}^{-c_0 t}.$

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Remark:

Hypocoercivity typically requires higher differentiation properties of the underlying PDE solution.

Variational interpretation

A key observation is a variational interpretation of hypocoercivity structures presented in G. ('21). Following this interpretation, we work as follows:

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We first test against $w\mathrm{e}^{-E}$ for $w \in H^1(\mu)$, to deduce

$$(u_t, w)_{L_2(\mu)} + (v \cdot \nabla_x u - \nabla V \cdot \nabla_v u, w)_{L_2(\mu)} + (\nabla_v u, \nabla_v w)_{L_2(\mu)} = 0.$$

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Next, we differentiate with respect to ∇_v:

$$\nabla_v u_t + \nabla_x u + (v \cdot \nabla_x)\nabla_v u - (\nabla V \cdot \nabla_v)\nabla_v u - \nabla_v \Delta_v u + \nabla_v u + (v \cdot \nabla_v)\nabla_v u = 0,$$

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and with respect to ∇_x:

$$\nabla_x u_t + (v \cdot \nabla_x)\nabla_x u - \mathcal{H}(V)\nabla_v u - (\nabla V \cdot \nabla_v)\nabla_x u - \nabla_x \Delta_v u + (v \cdot \nabla_v)\nabla_x u = 0,$$

with $\mathcal{H}(V)$ denoting the Hessian matrix of V with respect to the variables x.

Variational interpretation

Combining the last two identities into vector form, we have

$$\nabla_{v,x} u_t + (v \cdot \nabla_x)\nabla_{v,x} u + \begin{pmatrix} I & I \\ -\mathcal{H}(V) & 0 \end{pmatrix} \nabla_{v,x} u - (\nabla V \cdot \nabla_v)\nabla_{v,x} u$$

$$- \sum_{j=1}^{d} \nabla_{v,x} u_{v_j v_j} + (v \cdot \nabla_v)\nabla_{v,x} u = 0,$$

for $I \equiv id_{d\times d} \in \mathbb{R}^{d\times d}$.

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for $I \equiv id_{d\times d} \in \mathbb{R}^{d\times d}$. Testing now against $\mathcal{A}\nabla_{v,x} w \mathrm{e}^{-E}$, where $\mathcal{A} \in \mathbb{R}^{2d\times 2d}$ with

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for $\alpha, \beta, \gamma > 0$ to be determined below, along with some algebra gives

$$(\nabla_{v,x} u_t, \mathcal{A}\nabla_{v,x} w)_{L_2(\mu)} + ((v\cdot\nabla_x)\nabla_{v,x} u - (\nabla V\cdot\nabla_v)\nabla_{v,x} u, \mathcal{A}\nabla_{v,x} w)_{L_2(\mu)}$$

$$+ (\begin{pmatrix} \alpha I - \beta\mathcal{H}(V) & \alpha I \\ \beta I - \gamma\mathcal{H}(V) & \beta I \end{pmatrix}\nabla_{v,x} u, \nabla_{v,x} w)_{L_2(\mu)} + \sum_{j=1}^{d}(\nabla_{v,x} u_{v_j}, \mathcal{A}\nabla_{v,x} w_{v_j})_{L_2(\mu)} = 0,$$

Variational interpretation

Adding the two red identities yields: for almost every $t \in (0, t_f]$, find $u \in H^2(\mu)$, such that

$$(u_t, w)_{L_2(\mu)} + (\nabla_{v,x} u_t, \mathcal{A} \nabla_{v,x} w)_{L_2(\mu)} + a(u, w) = 0,$$

where

$$\begin{aligned} a(u, w) := {} & (v \cdot \nabla_x u - \nabla V \cdot \nabla_v u, w)_{L_2(\mu)} \\ & + ((v \cdot \nabla_x) \nabla_{v,x} u - (\nabla V \cdot \nabla_v) \nabla_{v,x} u, \mathcal{A} \nabla_{v,x} w)_{L_2(\mu)} \\ & + (\begin{pmatrix} (1+\alpha) I & \alpha I \\ \beta I & \beta I \end{pmatrix} \nabla_{v,x} u, \nabla_{v,x} w)_{L_2(\mu)} \\ & + \sum_{j=1}^{d} (\nabla_{v,x} u_{v_j}, \mathcal{A} \nabla_{v,x} w_{v_j})_{L_2(\mu)} \\ & - \beta (\mathcal{H}(V) \nabla_v u, \nabla_v w)_{L_2(\mu)} - \gamma (\mathcal{H}(V) \nabla_v u, \nabla_x w)_{L_2(\mu)}. \end{aligned}$$

The sign of the last two terms is unclear: $\mathcal{H}(V)$ is not definite...

Hypocoercivity

Lemma (Villani ('09))

Let $g \in H^1(\mu)$ *and energy* $E(v,x) = V(x) + \frac{1}{2}|v|^2$, *with* $V \in C^2(\mathbb{R}^d)$ *satisfying*

$$|\mathcal{H}(V)|_{Frob} \leq C_0(1 + |\nabla V|),$$

pointwise for all $x \in \mathbb{R}^d$. *Then, for* $C_1 := 16C_0^2(1+\sqrt{2dC_0})^2$, *we have*

$$\|\mathcal{H}(V)g\|_{L_2(\mu)}^2 \leq C_1\left(\|g\|_{L_2(\mu)}^2 + \|\nabla_x g\|_{L_2(\mu)}^2\right)$$

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$$\|\mathcal{H}(V)g\|^2_{L_2(\mu)} \leq C_1\left(\|g\|^2_{L_2(\mu)} + \|\nabla_x g\|^2_{L_2(\mu)}\right)$$

Lemma (Hypocoercivity)

For any $v \in H^3(\mu)$*, there exist* $\alpha, \beta, \gamma > 0$ *with* $\alpha\gamma - \beta^2 \geq 0$*, so that*

$$a(v,v) \geq c_{hc}\left(\|\nabla_v v\|^2_{L_2(\mu)} + \beta\|\nabla_x v\|^2_{L_2(\mu)}\right) + c_{hc,2}\alpha\|\nabla_v\nabla_v^T v\|^2_{L_2(\mu)} + c_{hc,3}\gamma\|\nabla_x\nabla_v^T v\|^2_{L_2(\mu)},$$

for positive constants $c_{hc,i}$*,* $i = 1,2,3$*, depending only on* C_1*.*

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Idea:

Employ discontinuous Galerkin (dG) inspired numerical flux functions for higher derivatives to retain the subtle algebraic structure.

- treat 4th order term à la Baker ('77), Engel et al. ('02), Brenner & Sung ('05), Feng & Karakashian ('05,'07)...
- conservative fluxes for odd order terms; Reed & Hill ('71), Yan & Shu ('02), Ayuso, Carillo & Shu ('12),....

A hypocoercivity-preserving Galerkin method

Semidiscrete method (fully discrete analysed): seek $U \in V_h$, s.t $\forall t \in (0, t_f]$

$$(U_t, W)_{L_2(\mu)} + (\nabla_{v,x} U_t, \mathcal{A} \nabla_{v,x} W)_{L_2(\mu)} + a_h(U, W) + s_h(U, W) = \ell(W),$$

for all $W \in V_h$, where

$$\begin{aligned} a_h(U, W) := {} & (v \cdot \nabla_x U - \nabla V \cdot \nabla_v U, W)_{L_2(\mu)} \\ & + ((v \cdot \nabla_x^h) \nabla_{v,x} U - (\nabla V \cdot \nabla_v^h) \nabla_{v,x} U, \mathcal{A} \nabla_{v,x} W)_{L_2(\mu)} \\ & + (\mathcal{B} \nabla_{v,x} U, \nabla_{v,x} W)_{L_2(\mu)} + \sum_{j=1}^{d} (\nabla_{v,x}^h U_{v_j}, \mathcal{A} \nabla_{v,x}^h W_{v_j})_{L_2(\mu)}. \end{aligned}$$

with

$$\mathcal{A} := \begin{pmatrix} \alpha I & \beta I \\ \beta I & \gamma I \end{pmatrix}, \qquad \mathcal{B} \equiv \mathcal{B}(V, \mathcal{A}) := \begin{pmatrix} (1+\alpha) I - \beta \mathcal{H}(V) & \alpha I \\ \beta I - \gamma \mathcal{H}(V) & \beta I \end{pmatrix}$$

A hypocoercivity-preserving Galerkin method

and $s_h : V_h \times V_h \to \mathbb{R}$ a stabilisation term, defined as

$$
\begin{aligned}
s_h(U,W) := \int_\Gamma \Bigg(& \frac{\nabla V \cdot n_v}{2}\Big(\alpha[\![\nabla_v U]\!]\cdot\{\!\{\nabla_v W\}\!\} + \beta[\![\nabla_v U]\!]\cdot\{\!\{\nabla_x W\}\!\}\Big) \\
& - \frac{v\cdot n_x}{2}\Big(\beta[\![\nabla_x U]\!]\cdot\{\!\{\nabla_v W\}\!\} + \gamma[\![\nabla_x U]\!]\cdot\{\!\{\nabla_x W\}\!\}\Big)\Bigg)\,\mathrm{d}\nu \\
& + \int_\Gamma \Big(\kappa\frac{|\nabla V\cdot \mathbf{n}_x|}{2}[\![\nabla_x U]\!]\cdot[\![\nabla_x W]\!] + \lambda\frac{|v\cdot\mathbf{n}_v|}{2}[\![\nabla_v U]\!]\cdot[\![\nabla_v W]\!]\Big)\,\mathrm{d}\nu \\
& - \sum_{j=1}^{d}\int_\Gamma \Big(\{\!\{\nabla_{v,x}^T U_{v_j}\}\!\}\mathcal{A}[\![\nabla_{v,x}W]\!]_{v_j} + \{\!\{\nabla_{v,x}^T W_{v_j}\}\!\}\mathcal{A}[\![\nabla_{v,x}U]\!]_{v_j} \\
& - \sigma[\![\nabla_{v,x}^T U]\!]_{v_j}\mathcal{C}[\![\nabla_{v,x}W]\!]_{v_j}\Big)\,\mathrm{d}\nu
\end{aligned}
$$

with $\mathcal{V} := (\nabla V^T, -v^T)^T$, for some $\kappa, \lambda > 0$ and $\mathcal{C}$ the stabilisation matrix with:

$$\sqrt{\mathcal{C}} = \left(\mathrm{diag}(\sqrt{\alpha} I, \sqrt{\gamma} I)\right)^{-1}\mathcal{A}$$

(consistency stability symmetrisation terms, respectively)

A hypocoercivity-preserving Galerkin method

To gain coercivity, thus, it remains to tame the Hessian $\mathcal{H}(V)$.

Lemma (Dong & G. (in prep.))

Let $g \in L_2(\mu) \cap H^1(\mu, \mathcal{T})$ and energy $E(v,x) = V(x) + \frac{1}{2}|v|^2$, with $V \in C^2(\mathbb{R}^d)$ with $|\mathcal{H}(V)|_{Frob} \leq C_0(1 + |\nabla V|)$, for $C_0 > 0$. Then, for $C_1 \equiv C_1(C_0)$, we have

$$\|\mathcal{H}(V)g\|^2_{L_2(\mu)} \leq C_1\big(\|g\|^2_{L_2(\mu)} + \|\nabla_x g\|^2_{L_2(\mu)}\big) + |\sum_{T\in\mathcal{T}} \int_{\partial T} \nabla V \cdot \mathbf{n}_x |g|^2 \,\mathrm{d}\nu.$$

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by selecting κ sufficiently large, we can tame the last term, to arrive at:

Hypocoercivity of the Galerkin bilinear form

Lemma

Select the function $\sigma : \Gamma \to \mathbb{R}$ *to be given by*

$$\sigma|_e := C_\sigma \mathrm{e}^{-E} p^2 |e| \max\left\{ \|\mathrm{e}^E\|_{L_\infty(T)} |T|^{-1}, \|\mathrm{e}^E\|_{L_\infty(T')} |T'|^{-1} \right\},$$

for each element face $e \subset \partial T \cap \partial T'$, $T, T' \in \mathcal{T}$, *for* $C_\sigma > 0$ *constant large enough. Then, there exist* $\alpha, \beta, \gamma > 0$ *with* $\alpha\gamma - \beta^2 \geq 0$ *s.t., for* $\kappa, \lambda \geq 0$ *large enough, we have*

$$\begin{aligned} a_h(W, W) + s_h(W, W) \geq\ & c_{hc} \left(\|\nabla_v W\|^2_{L_2(\mu)} + \beta \|\nabla_x W\|^2_{L_2(\mu)} \right) \\ & + c_{hc,2} \alpha \|\nabla_v^h \nabla_v^T W\|^2_{L_2(\mu)} + c_{hc,3} \gamma \|\nabla_x^h \nabla_v^T W\|^2_{L_2(\mu)} \\ & + \frac{1}{2} \sum_{j=1}^{d} \int_\Gamma \sigma |\sqrt{\mathcal{C}} [\![\nabla_{v,x} W]\!]_{v_j}|^2 \, \mathrm{d}\nu, \end{aligned}$$

for $c_{hc,i} > 0$, $i = 1, 2, 3$ *independent of* $\mathcal{T}$ *and* $\sqrt{\mathcal{C}} = \left(\mathrm{diag}(\sqrt{\alpha} I, \sqrt{\gamma} I) \right)^{-1} \mathcal{A}$.

Space discretisation

mass conservation of semidiscrete scheme

If finite element space V_h contains constants, we have

$$\int U \,\mathrm{d}\mu = \int u_0 \,\mathrm{d}\mu = \bar{u}, \quad t \in [0, t_f].$$

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Theorem (Decay via hypocoercivity)

There is a $\kappa > 0$, independent of h, p and U, such that, we have the bound

$$\|U(t_f) - \bar{u}\|^2_{L_2(\mu)} + \|\sqrt{\mathcal{A}}\nabla_{v,x} U(t_f)\|^2_{L_2(\mu)} \le \mathrm{e}^{-\kappa t_f}(\|U_0 - \bar{u}\|^2_{L_2(\mu)} + \|\sqrt{\mathcal{A}}\nabla_{v,x} U_0\|^2_{L_2(\mu)}).$$

Space-time discretisation

We can use, e.g., *hp*-version dG-timestepping:

for each time interval $I_n := (t_{n-1}, t_n]$, $n = 2, \ldots, N_t$, the solution $U|_{I_n} \in V^{\mathsf{p}}(I_n; \mathcal{T})$ is given by:

$$\begin{aligned} &\int_{I_n} \big((U_t, V) + (\nabla_{v,x} U_t, \mathcal{A} \nabla_{v,x} V) + a_h(U, V) + s_h(U, V) \big) \,\mathrm{d}t \\ &+ (U(t_{n-1}), V_{n-1}^{+}) + (\nabla_{v,x} U(t_{n-1}), \mathcal{A} \nabla_{v,x} V_{n-1}^{+}) \\ = \; &(U_{n-1}^{-}, V_{n-1}^{+}) + (\nabla_{v,x} U_{n-1}^{-}, \mathcal{A} \nabla_{v,x} V_{n-1}^{+}) \end{aligned}$$

for all $V \in V^{\mathsf{p}}(I_n; \mathcal{T})$, with $U_{n-1}^{-} := U(t_{n-1}^{-})$ and $U_0^{-} = u_0$.

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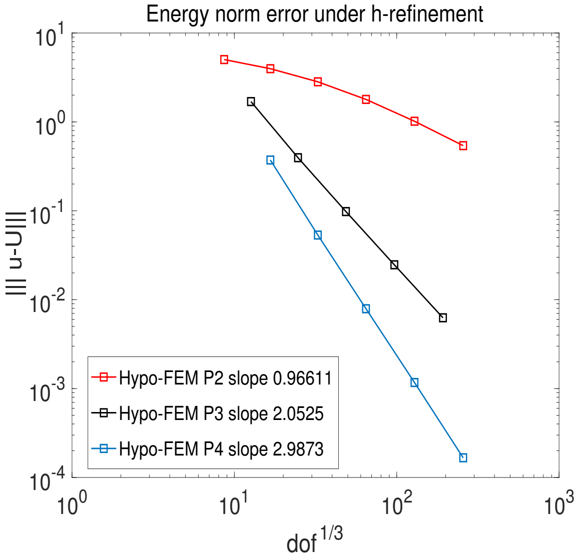
for all $V \in V^{\mathrm{p}}(I_n; \mathcal{T})$, with $U_{n-1}^- := U(t_{n-1}^-)$ and $U_0^- = u_0$.

hp-version a priori error analysis for the space-time method follows under a number of technical assumptions.

Convergence rate verification

$u_t - u_{xx} + xu_y = f$ for $t \in (0,1]$, with smooth known solution



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- Regularity/hypoellpticity of the dual of the spatial operator is unclear currently. No Aubin-Nitsche tricks as yet.
- The methodology is extremely general, allowing for construction of finite element methods for different hypocoercive PDEs of second order.

Conclusions

- A Galerkin framework for degenerate PDEs with special structure via hypocoercivity – important/relevant particular cases!
- hypocoercivity reinstates positivity to specially structured problems, in cases where the use of normal equations fails.
- Potentially allows porting of known theoretical and practical tools from elliptic and parabolic Galerkin methods to this class of degenerate PDEs.

— * —

E. H. Georgoulis
Hypocoercivity-compatible finite element methods for the long-time computation of Kolmogorov's equation
SIAM Journal on Numerical Analysis 59(1) pp.173-194 (2021)

Z. Dong & E. H. Georgoulis
Hypocoercivity-compatible Galerkin methods for inhomogeneous Fokker-Planck equations
In preparation.

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In this case, we define V_h to be a suitable reduced complexity space, e.g.,

- sparse grids / hyperbolic crosses Griebel ('05)
- sparse anisotropic Gaussians – MuSIK G., Levesley, Subhan ('10)
- TT, SVD, ...

such that they ensure the two crucial properties

$$V_h \subset H^1(\mu) \quad \text{and} \quad \{1\} \in V_h$$

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It is possible to make a two level (local–global) construction:

$$V_h := \tilde{\mathcal{P}}_q(\mathbb{R}^d \times \mathbb{R}^d) \oplus S_h$$

Spectral gap: criteria for Poincaré inequalities

Theorem

Let $V \in C^2(\mathbb{R}^d)$ *such that* e^{-V} *is a probability density on* $\mathbb{R}^d$*. If also*

$$\frac{1}{2}|\nabla V(x)|^2 - \Delta V(x) \to \infty,$$

as $|x| \to \infty$*, then* $\mu := \mathrm{e}^{-V}\,\mathrm{d}x$ *satisfies a Poincaré inequality.*