Multiscale Phenomena and Singularity in Fluids: Computation and Analysis

Yixuan (Roy) Wang*

Caltech ACM
roywang@caltech.edu

Candidacy Talk

May 11, 2023

Summary of our contribution: ExpMsFEM

Systematic approach for solving multi-query multiscale problems efficiently using **offline bases**, with state-of-the-art accuracy **rigorously**.

- For elliptic equations: *Multiscale Modeling & Simulation* 2021
- For Helmholtz equations: *Multiscale Modeling & Simulation* 2023
- Review paper: *Communications on Applied Mathematics and Computation* 2023

Joint work with Chen, Hou.
Ongoing collaboration on generalization to the Schrödinger equation.

Multiscale model reduction

- **Model problem** in 2D and 3D:

$$-\nabla \cdot (A(x)\nabla u) - P(x)u = f, \text{ in } \Omega \subset \mathbb{R}^d, \quad \text{w/ boundary conditions}$$

wave mechanics, subsurface flows, electrostatics, seismology.

  - Heterogeneity: $A, P \in L^\infty(\Omega)$ without scale separation. $0 < A_{\min} \leq A(x) \leq A_{\max}$. $f \in L^2(\Omega)$.
  - Highly **Oscillatory** solutions.

- **Model reduction**: use a small number of local basis functions to achieve desired **accuracy theoretically and numerically**.
  - Desirable if same offline bases can be used with different f.

Literature on multiscale methods for elliptic equations

- **Local** bases + **global** coupling
  - Multiscale Finite Element Methods (MsFEM): Hou, Wu 1997
  - Genealized Finite Element Methods (GFEM) via Partition of Unity Method (**PUM**): Babuska, Lipton 2011
- **Global** bases via variational problem + **local** truncation
  - Gamblets: Owhadi-Zhang-Berlyand 2014
  - Localizable Orthogonal Decompositions (**LOD**): Malqvist, Peterseim 2014
- VMS 1998, HMM 2003...

Helmholtz equation and pollution effect

Helmholtz equation with high wave number k:

$$\mathcal{L}_k u := -\nabla \cdot (A\nabla u) - k^2V^2u = f, \text{ in } \Omega, \quad \text{w/ boundary conditions}$$

where $V \in L^\infty(\Omega)$.

- Numerical difficulty: **pollution effect** (Babuska, Sauter 1997)
  - Maximal mesh size to address the wave length: $O(1/k)$.
  - Standard FEM: local mesh size $H = O(1/k^2)$.
  - Ideal method: $H = O(1/k)$!
- Mathematical challenge: **indefinite** operator.

Overcoming the pollution effect

Two key insights and methods that capture oscillation with $O(H)$ error

- **Gårding-type inequality**: good approximation implies good solution. $hp-$FEM with polynomial of order $O(\log k)$. (Melenk, Sauter 2010)

- **Poincaré inequality**: local problem resembles elliptic problem. LOD with support size $O(H\log(1/H)\log k)$. (Peterseim 2017)

Our method: Best of (G) and (P)

- ExpMsFEM with first exponential rate of convergence. (C-H-W)

- Later: PUM with same rate of convergence. (Ma-Alber-Scheichl)

Four methods have comparable complexity if aimed at minimal accuracy: $O(1/k)$ error in **energy norm**, mesh size $O(1/k)$, DoF $O(k^d\text{poly}(\log(k)))$.

Explore the solution space (G)

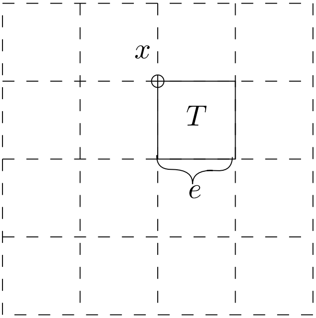
- **Mesh structure** in 2D:
  nodes, edges and elements.

- **Split** the solution locally (P):
  in each T, $u = u_T^{\mathsf{h}} + u_T^{\mathsf{b}}$.

$$\begin{cases} \mathcal{L}_k u_T^{\mathsf{h}} = 0 \ \text{ in } T \\ \quad u_T^{\mathsf{h}} = u \ \text{ on } \partial T, \end{cases}$$

$$\begin{cases} \mathcal{L}_k u_T^{\mathsf{b}} = f \ \text{ in } T \\ \quad u_T^{\mathsf{b}} = 0 \ \text{ on } \partial T. \end{cases}$$

- **Merge**: For each T, $u^{\mathsf{h}}(x) = u_T^{\mathsf{h}}(x)$ and $u^{\mathsf{b}}(x) = u_T^{\mathsf{b}}(x)$, when $x \in T$.



$x \in \mathcal{N}_H, e \in \mathcal{E}_H, T \in \mathcal{T}_H$

Key insights of exponential accuracy

- (Generalized) **harmonic-bubble splitting** (Hetmaniuk, Lehoucq 2010), (Hou, Liu 2016)
- **Edge localization**
- **Oversampling** (Hou, Wu 1997) for low-complexity edge space

Theorem (Informal statement of exponentially efficient edge bases)

Suppose $H = O(1/k)$, then for each edge e, we can find m local edge bases such that the relative error using those edge bases to approximate any edge function is at most $C \exp\left(-bm^{\frac{1}{d+1}}\right)$.

Sketch of our result

On a mesh of lengthscale $H = O(1/k)$, u can be computed by

$$u = \underbrace{\sum_{i \in I_1} c_i^f \psi_i^{(1)}}_{\text{(I)}} + \underbrace{\sum_{i \in I_2} \psi_i^f}_{\text{(II)},O(H)} + C \exp(-b m^{\frac{1}{d+1}}) \qquad \text{(Energy norm)}$$

b, C constants independent of H, k. $\psi_i^{(1)}, \psi_i^f$ *local* support of size H.

- $\psi_i^{(1)}$ via *local* SVD of $\mathcal{L}_k$, offline, parallelizable $\quad \#I_1 = O(m/H^d)$
- ψ_i^f via solving *locally* $\mathcal{L}_k u = f$ online, parallelizable $\quad \#I_2 = O(1/H^d)$
- c_i^f obtained by Galerkin methods with bases $\psi_i^{(1)}$; offline matrix

A data-adaptive coarse-fine scale decomposition

Artificial example with rough media and high wavelength

Rough media, high wavelength $k = 2^5$ with mixed boundary conditions.

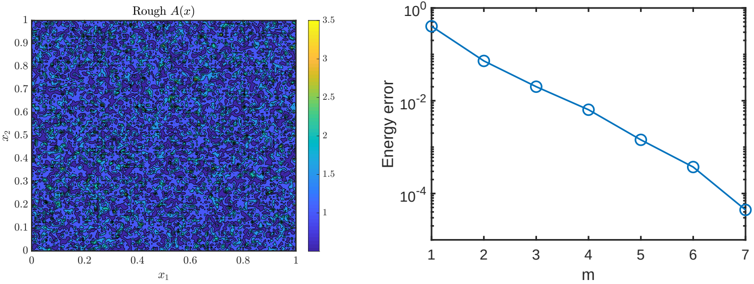


Figure: Left: the contour of A; right: relative errors in the energy norm.

Exponential decaying error; works better in practice than PUM.

Backup example of high wavenumber

- $A = V = \beta = 1$, $k = 2^7$, fine mesh $h = 2^{-10}$, coarse mesh $H = 2^{-5}$.
- Exact solution: $u(x_1, x_2) = \exp(-ik(0.6x_1 + 0.8x_2))$.

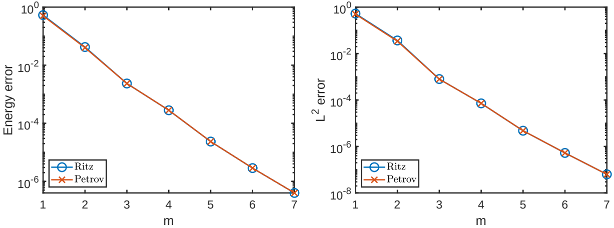


Figure: High wavenumber example. Left: $e_{\mathcal{H}}$ versus m; right: e_{L^2} versus m.

Backup example of high contrast: Mie resonances

$$\Omega_\varepsilon = (0.25, 0.75)^2 \cap \bigcup_{j\in\mathbb{Z}^2} \varepsilon\left(j + (0.25,0.75)^2\right), \quad A(x) = \begin{cases} 1, & x \notin \Omega_\varepsilon \\ \varepsilon^2, & x \in \Omega_\varepsilon \,. \end{cases}$$

$\beta = 1, V = 1, k = 9.$

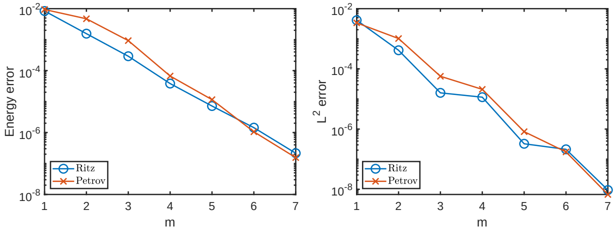


Figure: High contrast example. Left: $e_{\mathcal{H}}$ versus m; right: e_{L^2} versus m.

Millennium prize problem: blowup of 3D NS equation

- 3D incompressible Navier-Stokes equation:

$$\mathbf{u}_t + \mathbf{u}\cdot\nabla\mathbf{u} = -\nabla\mathbf{p} + \nu\Delta\mathbf{u}, \quad \nabla\cdot\mathbf{u} = 0\,. \tag{1}$$

- Euler equation: $\nu = 0$. NS equation $\nu > 0$.
- Blowup of a quantity of interest f:

$$\limsup_{t\to T^-} \|f(t)\|_{L^\infty} = \infty, \quad T < +\infty\,.$$

- Millennium prize problem: global well-posedness or finite time blowup of (1) from **smooth** initial data **on the whole space**.

Self-similar blowup and axisymmetric equation

- **Structured** singularity with less DoF
  - **Self-similar** blowup:

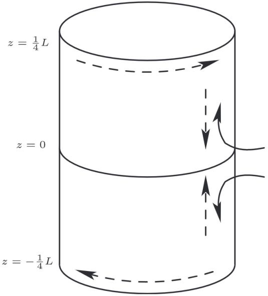
$$f(t,\mathbf{x}) = (T-t)^{c_f} F(\mathbf{x}/(T-t)^{c_l})\,. \tag{2}$$

    T: blowup time; $c_f < 0$: blowup rate.
  - **Axisymmetric** Euler equation: cylindrical formulation (r, z, θ), velocity independent of θ.

- Hou-Luo 2013 : numerical evidence of self-similar blowup for **smooth** initial data of 3D axisymmetric Euler equation with **boundary**.
  Chen-Hou 2022 : rigorous proof of blowup.

Self-similar blowup candidates of 3D axisymmetric Euler

- Blowup on the **boundary** for H-L case



Boundary helps blowup!

- **Our goal**: identify and understand blowup in the **interior**
  - (equivalently) Approaching millennium prize problem.
  - Generalize blowup mechanism from 1D to 3D.

1D models with self-similar blowup: gCLM

- Vorticity formulation $\boldsymbol{\omega} = \nabla \times \mathbf{u}$ for 3D Euler:

$$\boldsymbol{\omega}_t + (\mathbf{u} \cdot \nabla)\boldsymbol{\omega} = \nabla \mathbf{u} \cdot \boldsymbol{\omega} \,. \tag{3}$$

- Biot-Savart law, $\boldsymbol{\omega} \to \mathbf{u}$ via nonlocal interaction: $\nabla \mathbf{u} = \mathcal{R}(\boldsymbol{\omega})$.
  $\mathcal{R}$: Riesz transform.

- 1D model: generalized CLM model (Okamoto-Sakajo-Wunsch 2008):

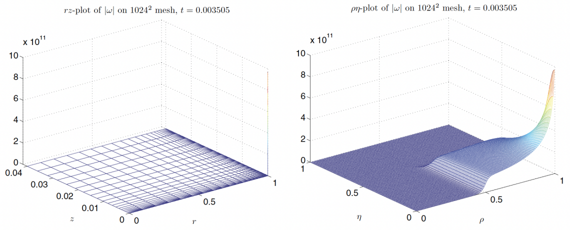
$$\omega_t + au\omega_x = u_x\omega, \quad u_x = H\omega \,. \tag{4}$$

  H: Hilbert transform, 1D analogue of Riesz transform.
  a: strength of **advection** in competition with **vortex stretching**.

Singularity: numerical computation

$$\limsup_{t\to T^-} \|\mathbf{f}(t)\|_{L^\infty} = \infty, \quad T < +\infty\,.$$

1. Physical equation: compute "infinity"! Adaptive mesh in Hou-Luo.



(a) rz-plane (b) $\rho\eta$-plane

2. Profile equation: $\mathbf{f}(t,\mathbf{x}) = (T-t)^{c_\mathbf{f}}\mathbf{F}(\mathbf{x}/(T-t)^{c_l})$. Finite $\mathbf{F}$.

Dynamic rescaling formulation

- **Profile equation** for 1d gCLM model $\omega_t + au\omega_x = u_x\omega$. Plugging in

  $$\omega(t,x) = (T-t)^{c_\omega}\Omega(x/(T-t)^{c_l})\,, u(t,x) = (T-t)^{c_\omega+c_l}U(x/(T-t)^{c_l})$$

  the self-similar ansatz and balance the terms in t, we get:

  $$(c_l y + aU)\,\Omega_y = (c_\omega + U_y)\,\Omega, \quad U_y = H\Omega\,. \tag{5}$$

- **Dynamic rescaling formulation** (DRF) for time-depedent c_l, c_ω:

  $$\Omega_\tau + (c_l y + aU)\,\Omega_y = (c_\omega + U_y)\,\Omega, \quad U_x = H\Omega\,. \tag{6}$$

  Equivalent to original equation by time rescaling.
  Steady state recovers profiles.
  Finite time blowup holds if $c_\omega \leq -C < 0$ and is self-similar if Ω, U converge to a profile.

Literature review on DRF

- Modulation technique (dispersive equations):
  - Nonlinear Schrödinger equation: McLaughlin-Papanicolaou-Sulem-Sulem 1986
  - Nonlinear wave equation: Merle, Zaag 2015
  - Nonlinear heat equation: Merle, Raphael 1997
  - Generalized KdV equation: Martel-Merle-Raphael 2014
- Fluid dynamics:
  - De Gregorio 1D model: Chen-Hou-Huang 2021
  - 2D Boussinesq and 3D Euler with $C^{1,\alpha}$ data: Chen-Hou 2020
  - 2D Boussinesq and 3D Euler with smooth data: Chen-Hou 2022

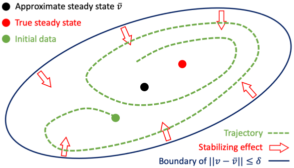
Framework of establishing self-similar blowup

1. Approximate profile: explicit construction; solving DRF/ profile.

Framework of establishing self-similar blowup

1. Approximate profile: explicit construction; solving DRF/ profile.

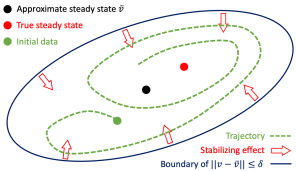
2. **Stability**: all initial data close to the approximate profile would develop finite-time blowup, i.e. the blowup is stable.
   - Weighted L^2 estimate or L^∞ estimate using characteristics.
   - **Rigorous proof**: interval arithmetic of numerical verifications.



Framework of establishing self-similar blowup

1. Approximate profile: explicit construction; solving DRF/ profile.

2. **Stability**: all initial data close to the approximate profile would develop finite-time blowup, i.e. the blowup is stable.
   - Weighted L^2 estimate or L^∞ estimate using characteristics.
   - **Rigorous proof**: interval arithmetic of numerical verifications.



3. Characterization of the blowup: rate, regularity, asymptotics...

Conjecture on blowup regularity of CCF model

CCF model (Cordoba-Cordoba-Fontelos 2005):

$$\omega_t - u\omega_x = u_x\omega, \quad u_x = H\omega\,. \tag{7}$$

Conjecture (Conjecture on blowup regularity (Silvestre, Vicol 2016))

Until blowup time, the solution of (7) will have bounded $C^{-1/2}$-norm.

Our work: (ongoing with Chen, Hou) Construction of a specific self-similar profile disproving the conjecture.

- Smooth profiles do not violate the conjecture numerically.
- Constructed profile $\omega = O(x^{7/6})$ near the origin.

A more faithful 1D model: Hou-Li

- N-S equation in axisymmetric case:

$$\begin{aligned} u_{1,t} - r\psi_{1,z}u_{1,r} + (2\psi_1 + r\psi_{1,r})u_{1,z} &= 2u_1\psi_{1,z} + \nu\Delta u_1 \,, \\ \omega_{1,t} - r\psi_{1,z}\omega_{1,r} + (2\psi_1 + r\psi_{1,r})\omega_{1,z} &= \left(u_1^2\right)_z + \nu\Delta\omega_1 \,, \\ -\left[\partial_r^2 + (3/r)\partial_r + \partial_z^2\right]\psi_1 &= \omega_1 \,. \end{aligned} \tag{8}$$

- Hou-Li (2008) constant approximation in r-direction:

$$\begin{aligned} u_t + 2\psi u_z &= 2u\psi_z + \nu u_{zz} \,, \\ \omega_t + 2\psi\omega_z &= \left(u^2\right)_z + \nu\omega_{zz} \,, \\ -\psi_{zz} &= \omega \,. \end{aligned} \tag{9}$$

- Model is well-posed in C^1; convection is weaker in 3D.

Our result on Hou-Li model

Weak convection model:

$$\begin{aligned} u_t + 2a\psi u_x &= 2u\psi_x + \nu u_{xx}\,, \\ \omega_t + 2a\psi\omega_x &= \left(u^2\right)_x + \nu\omega_{xx}\,, \\ -\psi_{xx} &= \omega\,. \end{aligned} \tag{10}$$

Our work: (forthcoming paper with Hou)

Theorem (Blowup of (10) with periodicity in x)

There exists steady blowups with scaling index in space $c_l = 0$, for

1. $a < 1$ *close to* 1, $\nu = 0$, *self-similar blowup with smooth data;*
2. $a < 1$ *close to* 1, $\nu > 0$, *blowup with smooth data;*
3. $a = 1$, $\nu = 0$, *self-similar blowup with any Hölder* $\alpha < 1$ *regularity.*

Proof of linear stability

- Explicit approximate profiles: from the steady state for $a = 1$.

$$(\bar{\omega}, \bar{u}, \bar{\psi}) = (\sin x, \sin x, \sin x).$$

- Linear stability for the perturbation:

$$D := \frac{1}{2}\frac{d}{dt}(\|u\|_{\chi_1}^2 + \|\omega\|_{\chi_2}^2) \approx (L_1, u)_{\chi_1} + (L_2, \omega)_{\chi_2} \lesssim -[\|u\|_{\chi_1}^2 + \|\omega\|_{\chi_2}^2] .$$

$$L_1 = -2\sin x u_x - 2\cos x\psi + 2u\cos x + 2\sin x\psi_x \,,$$

$$L_2 = -2\sin x\omega_x - 2\cos x\psi + 2u\cos x + 2\sin x u_x \,.$$

- Singular weights: $\rho_0 = \frac{1}{1-\cos x}, \rho_k = (1+\cos x)^k$ with the norm

$$E_k^2(t) = (u^{(k+1)}, u^{(k+1)}\rho_k) + (\omega^{(k)}, \omega^{(k)}\rho_k) \,.$$

Damping in the leading order term.

Difficulties in linear estimate

- Estimate of local and nonlocal terms in L^2:

$$D_0 = -\left[(u_x, u_x\rho) + (\omega, \omega\rho) + (u, u\rho)\right] + 2\left[-(\cos x\psi, \omega\rho) + (\sin x\psi, u_x\rho) + (u\cos x, \omega\rho)\right].$$

- **Exact** computation in Fourier basis to avoid overestimate.
- Establish negative-definiteness of **quadratic form** (w.r.t Fourier coefficients) with decaying entries.
- **Computer-assisted verification** of finite truncation: the quadratic form projected in first 200 basis.

Backup slide: difficulties in viscous terms

- H^k estimates for the viscous term spit out for example

$$(\omega^{(k+2)}, \omega^{(k)}\rho_k) \approx -(\omega^{(k+1)}, \omega^{(k+1)}\rho_k) + C(k)(\omega^{(k)}, \omega^{(k)}\rho_{k-1}) \,.$$

- Criteria for the norm:
  - Linear damping
  - Stronger than $W^{3,\infty}$-norm near the origin
  - Control on viscous terms

- Combination of a cascade of norms to close the estimate:

$$I^2 = \sum_{k=0}^{4} E_k^2 \mu^k \,, \quad \mu \ll 1 \,.$$

Comparison of numerical methods

1. Adaptive mesh for physical equation: problem specific methods, under-resolution, requires scaling and fitting, only stable profile.

Comparison of numerical methods

1. Adaptive mesh for physical equation: problem specific methods, under-resolution, requires scaling and fitting, only stable profile.

2. DRF equation: problem specific methods, solves for profiles, only stable profile, high accuracy.

Comparison of numerical methods

1. Adaptive mesh for physical equation: problem specific methods, under-resolution, requires scaling and fitting, only stable profile.
2. DRF equation: problem specific methods, solves for profiles, only stable profile, high accuracy.
3. NN based approach for profile (PINN/PINO): generic method, solves for profiles, unstable profile? high accuracy?
   - Wang-Lai-Gomez-Buckmaster 2022: PINN for 2D Boussinesq profile.
   - Our work: *Neurips workshop* 2022 and forthcoming paper with Maust, Li et al., on generalizing Fourier Neural Operators to non-periodic problems in 1D and higher dimensions.

Blowup beyond self-similar setting

- Numerical evidence by Hou on 3D Euler/N-S interior singularity: **two-scale** blowup phenomena, differing by a logarithmic correction.
  - Increase ambient dimension to ≈ 3.1 to observe self-similar blowup.
- We studied non self-similar blowups in modified Burgers' equation.
- Other models with $\log$ corrections: hydrostatic Euler equation, nonlinear Schrödinger equation, 2D Keller-Segel equation...

Future work

- Singularity formulation:
  - Introduce frameworks to study **mathematically and numerically** blowup with $\log$-like corrections.
  - Optimization-based methods (PINNs) to solve **numerically** blowups unstable in DRF: vary the **dimension** and identify a blowup with scaling matching the theoretical scaling for N-S.
- Multiscale problems: numerical experiment for **higher dimensions**; theory for **higher-order operators**; **operator learning** for solving local problems.

Backup example: Keller-Segel equation

- 2D Keller-Segel equation, describing chemotaxis in biology

$$\begin{cases} \partial_t u = \Delta u - \nabla \cdot (u \nabla \Phi_u)\,, & \text{in } \mathbb{R}^2 \\ 0 = \Delta \Phi_u + u\,. \end{cases}$$

- Mass preservation; blowup when $M > 8\pi$.
- Stationary profile: $Q(x) = \frac{8}{(1+|x|^2)^2}$.
- Self-similar variables:

$$u(x,t) = \frac{1}{T-t} w(z,\tau), \quad z = \frac{x}{\sqrt{T-t}}, \quad \frac{d\tau}{dt} = \frac{1}{T-t}\,,$$

$$\partial_\tau w = \nabla \cdot (\nabla w - w \nabla \Phi_w) - \frac{1}{2} \nabla \cdot (zw).$$

Backup example: Keller-Segel equation

- Blowup variables:

$$w(z,\tau) = Q_\nu(z) + \eta(z,\tau),\ \text{where } Q_\nu(z) = \frac{1}{\nu^2} Q\left(\frac{z}{\nu}\right),$$

while the next-order term η solves

$$\partial_\tau \eta = \mathcal{L}^\nu \eta + \left(\frac{\nu_\tau}{\nu} - \frac{1}{2}\right) \nabla \cdot (zQ_\nu) - \nabla \cdot (\eta \Phi_\eta), \quad \nu \to 0 \text{ unknown},$$

- Final result: (Collot-Ghoul-Masmoudi-Nguyen 2021)

$$u(x,t) = \frac{1}{\lambda^2(t)} \left[Q\left(\frac{x-a(t)}{\lambda(t)}\right) + \varepsilon(x,t) \right],$$

$$\lambda(t) \sim 2e^{-\frac{\gamma+2}{2}} \sqrt{T-t} \exp\left(-\frac{\sqrt{|\log(T-t)|}}{\sqrt{2}}\right).$$