Hybrid Methods for Complex Particle Systems

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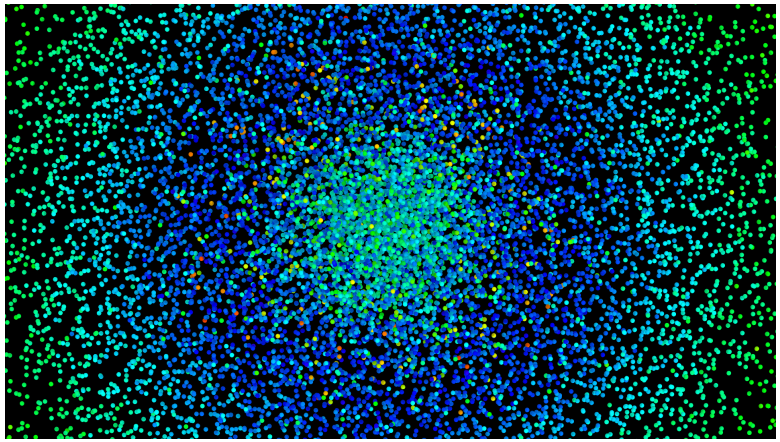

Advanced Scientific Computing Advisory Committee Meeting

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Project summary

This project is dedicated to the development of hybrid, hierarchical, and multi-level algorithms for the simulation of complex many-particle systems. These systems form key components in a variety of energy generation and energy storage devices. Example applications include gas dynamics, plasmas, radiation, multiphase flows, and charge transport in materials. The challenge in simulating particle systems is one of computational complexity, a consequence of the huge number of unknowns in the system and the large variations in temporal and spatial scales over which they evolve. We tackle this challenge through the use of hybrid methods which leverage reduced models, when they are valid, to increase the efficiency of simulations, thereby freeing computational resources to resolve important fine scale features. This effort relies on the central role played by kinetic models that, unlike fluid descriptions, can capture non-equilibrium behavior, but approximate detailed information about particle correlations stochastically via collision operators. The first goal of the project is to use the dissipative structure of these operators to connect the fluid and kinetic descriptions in a single efficient method for attacking multiscale problems. The second goal is to improve the efficiency of molecular dynamics solvers using the solution of the kinetic model as a preconditioner.

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From particles to fluids

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What are many-particle systems?

- A *many-particle system* (or *many-body system*) is a collection of a large number of individual objects that interact with each other and/or with the external environment.
- "Particles" can be molecules, ions, electrons, neutrons, photons, phonons, cells, micro-organisms, human beings, cars, stocks, packets of data, memes, ...
- Classical objects (no quantum mechanics or relativity).
- **Multi-scale phenomena:** Collective or competing processes at the microscopic level induce behavior on macroscopic scales.

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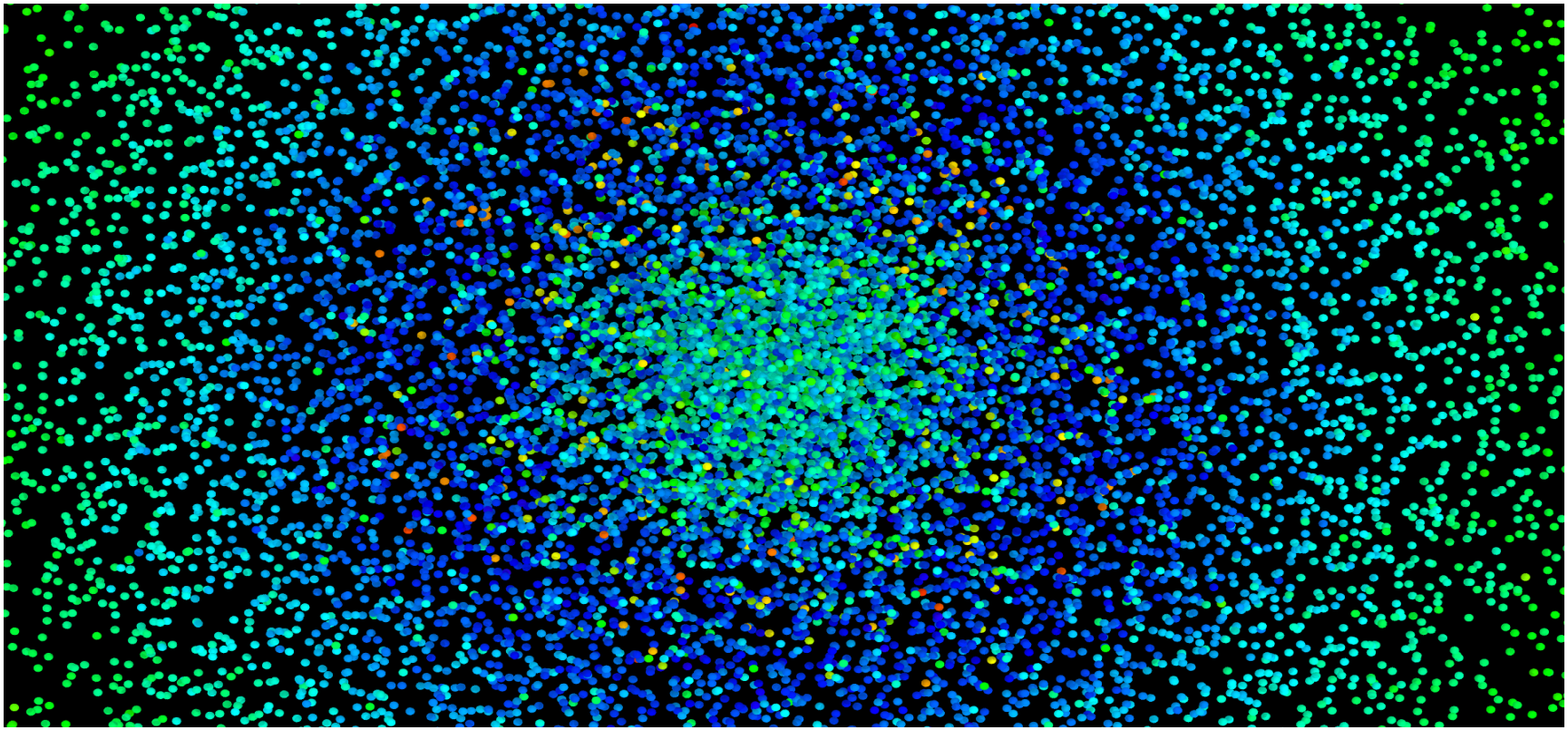
Motivational example: a "hollow plasma"



Video courtesy of
Professor Michael Murillo and Dr. Vikram Dharodi,
Michigan State University

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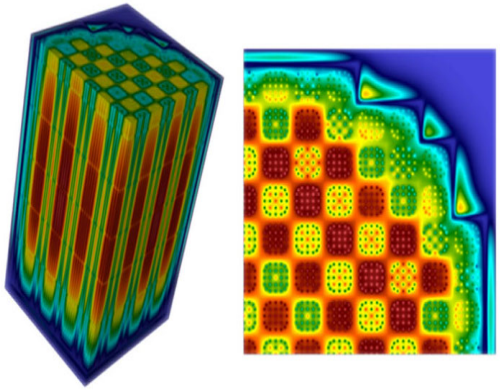
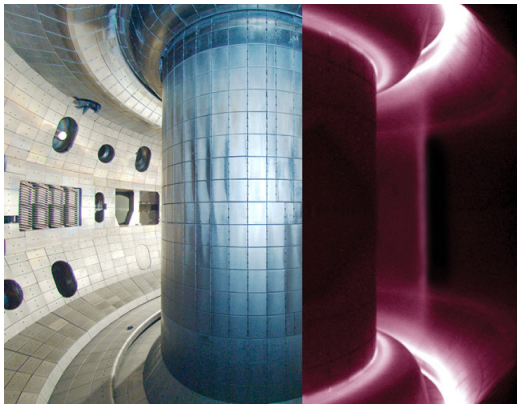
Applications important to DOE



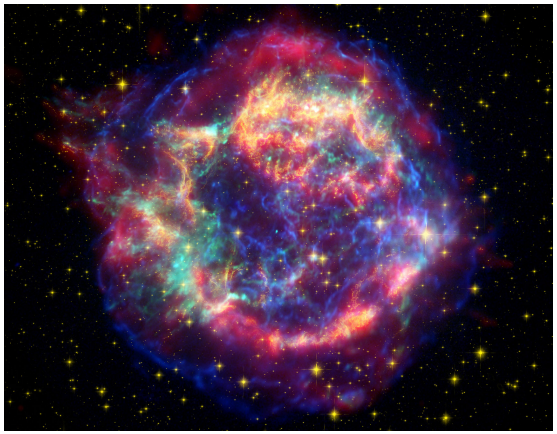
(a) fission reactors



(b) fusion reactors

(c) photovoltaic devices

(d) gasification



(e) HEDP and NP

(f) stockpile stewardship

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The challenge of complex systems

> *The underlying physical laws necessary for the mathematical theory of a large part of physics ... are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.*
>
> –Paul Dirac, Proceedings of the Royal Society of London, 1926

1. Even if we understand microscopic dynamics, we don't (and often won't) have enough computing power.
   - Too many unknowns
   - Not enough resolution
2. The macroscopic features that we care about are driven by microscopic dynamics.

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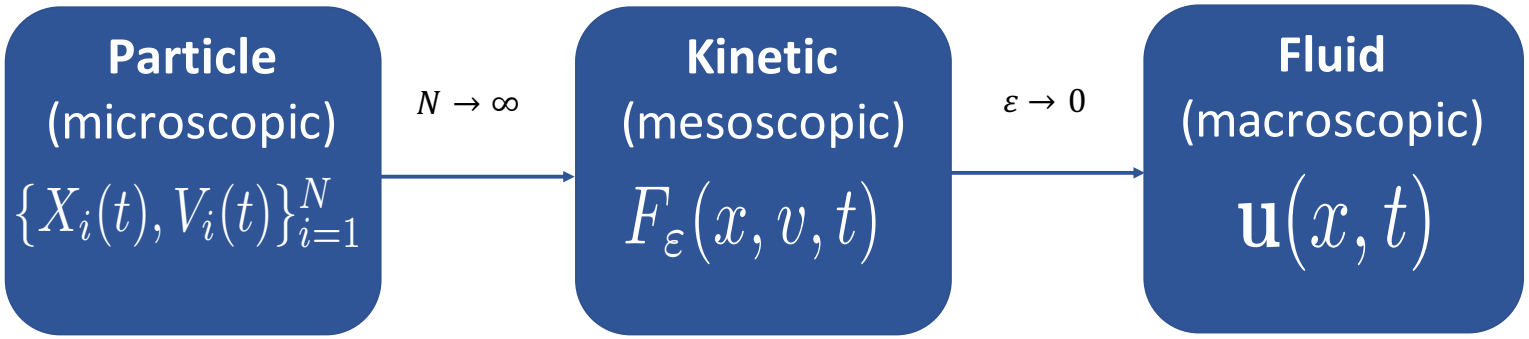
The kinetic description of particle systems

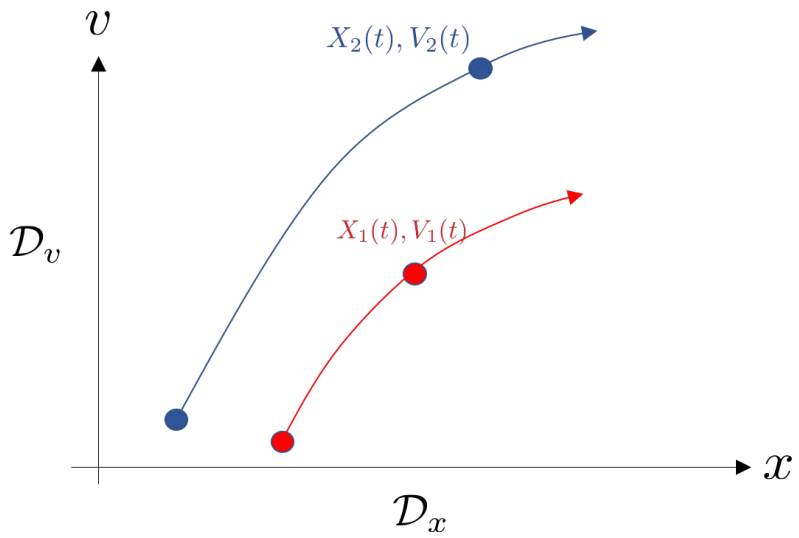
> *It seems to me desirable [to pursue] a rigorous and satisfactory development of the method of mean values in mathematical physics, and in particular in the kinetic theory of gases.... Boltzmann's work on the principles of mechanics suggests the problem of developing mathematically the limiting processes ... which lead from the atomistic view to the laws of motion of continua.*
>
> –David Hilbert, International Congress of Mathematicians, Paris, 1900

For gases, kinetic equations provide an intermediate model between particle and fluid descriptions.



The particle description

A system of N particles is characterized by positions $\mathbf{X} = \{X_1, \ldots, X_N\}$ and velocities $\mathbf{V} = \{V_1 \ldots, V_N\}$.



The vectors $\mathbf{X}$ and $\mathbf{V}$ satisfy a sytem of coupled ordinary differential equations.

$$\dot{\mathbf{X}}(t) = \mathbf{V}(t) \qquad \dot{\mathbf{V}}(t) = \mathbf{A}(\mathbf{X}(t), \mathbf{V}(t))$$

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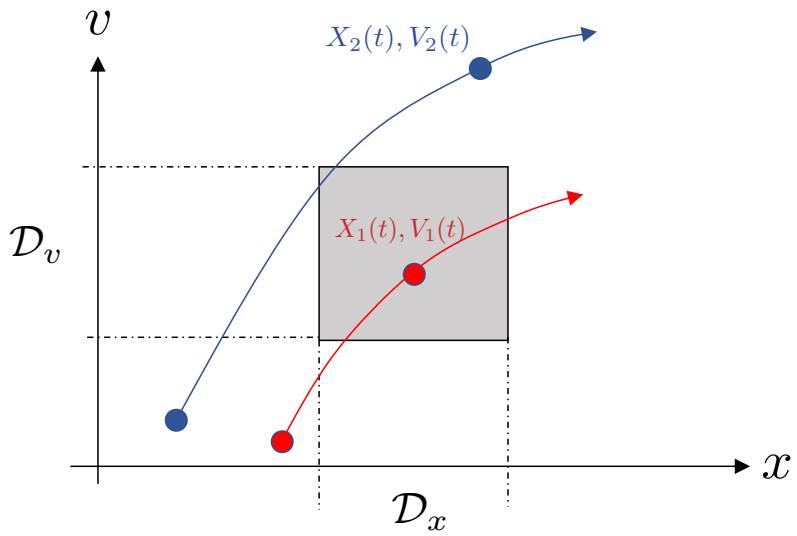
The kinetic description

The *kinetic distribution function* F is defined such that

$$\int_{\mathcal{D}_x} \int_{\mathcal{D}_v} F(x, v, t) dv dx$$

gives the number of particles is the phase space volume $\mathcal{D}_v \times \mathcal{D}_x$.



The kinetic equation for F is

$$\boxed{\partial_t F + v \cdot \nabla_x F + a[F] \cdot \nabla_v F = \mathcal{C}[F]}$$

where a is the particle acceleration to global fields and the *collision operator* $\mathcal{C}$ is an integral operator that models particle interactions.

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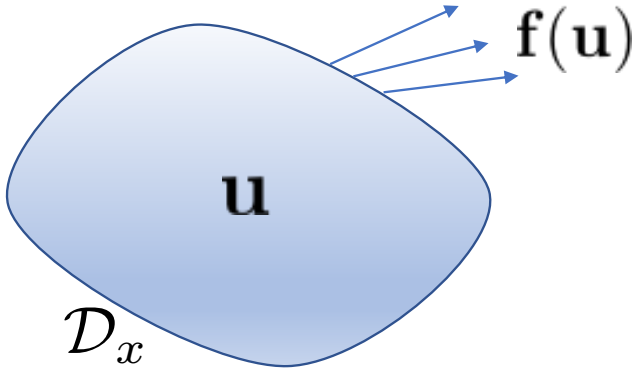
The fluid description

Fluid variables $\mathbf{u} = (u_1, u_2, \ldots, u_n)$ are quantities of interest defined such that

$$\int_{\mathcal{D}_x} u_i(x,t)dx, \quad i = 1, \ldots, n$$

gives the amount of some quantity of interest (e.g. mass, momentum, energy) contained inside $\mathcal{D}_x$ at time t.



Fluid equations take the form

$$\boxed{\partial_t \mathbf{u} + \nabla_x \cdot \mathbf{f}(\mathbf{u}) = \mathbf{r}(\mathbf{u})}$$

where $\mathbf{f}$ describes the flux of $\mathbf{u}$ across a boundary and $\mathbf{r}$ describes gains and loss due to mixing and interactions with the surrounding environment.

Examples of fluid equations include Euler, Navier-Stokes, diffusion, drift-diffusion, and magnetohydrodynamics (MHD).

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From particles to fluids

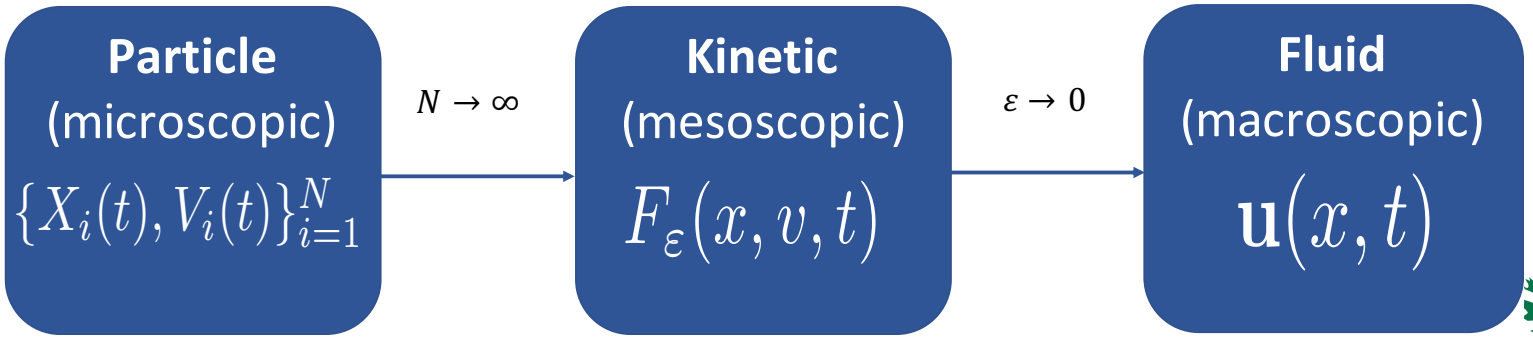
- **Particle $\to$ kinetic.** The particle description recovers to the kinetic decription as the particle number $N \to \infty$, assuming inter-particle forces become
  1. Weaker (acceleration due to global fields) and/or
  2. Highly localized (collision operator)

  This limit is not valid for solids or liquids.

- **Kinetic $\to$ fluid.** As $\varepsilon \to 0$, $F = F_\varepsilon$ converges to a local thermal equilibrium

$$F_\varepsilon(x, v, t) \xrightarrow{\varepsilon \to 0} \mathcal{M}[\mathbf{u}(x,t)](v) \tag{1}$$

  where $\mathcal{M}[\mathbf{u}]$ is a known function of v that is parameterized by fluid variables $\mathbf{u}$.



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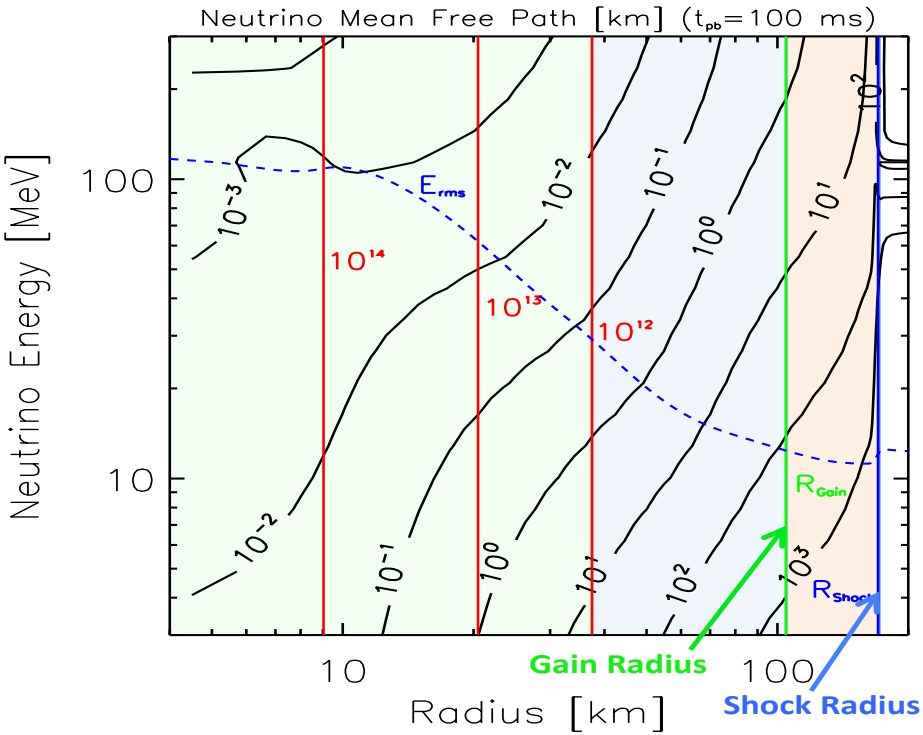
The physical meaning of ε

- The parameter ε is called the *Knudsen number*:

$$\varepsilon = \frac{\text{mean free path}}{\text{domain length}}$$

It may vary by several orders of magnitude in a single problem.



Above: supernova simulation with $10^{-5} \lesssim \varepsilon \lesssim 10^{1}$.

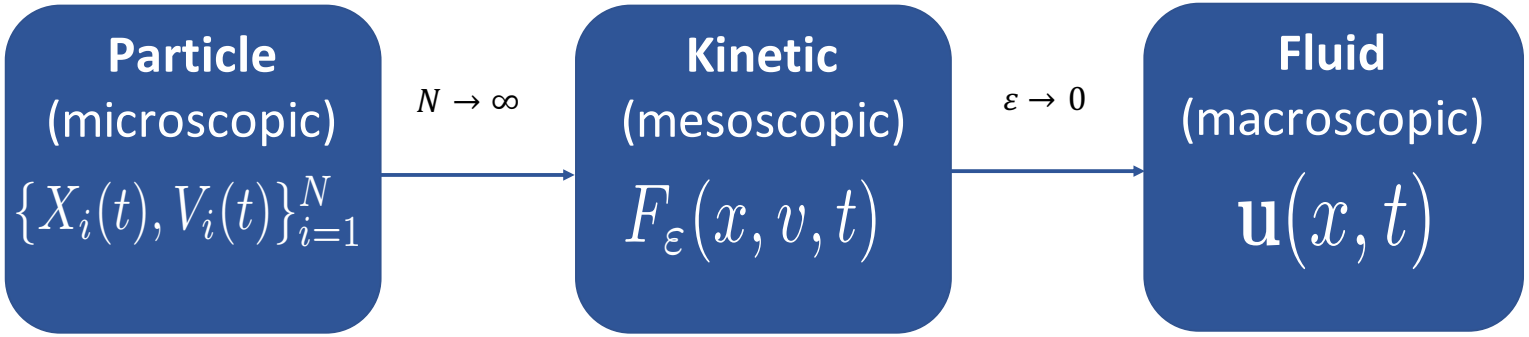
A high-level view of the project

Project goals

1. Connect the fluid and kinetic descriptions in a single efficient method for attacking multiscale problems. This is (2/3) of the effort.

2. Improve the efficiency of molecular dynamics solvers using the solution of the kinetic model as a preconditioner. This is (1/3) of the effort.

Effort so far has focused on the first goal.



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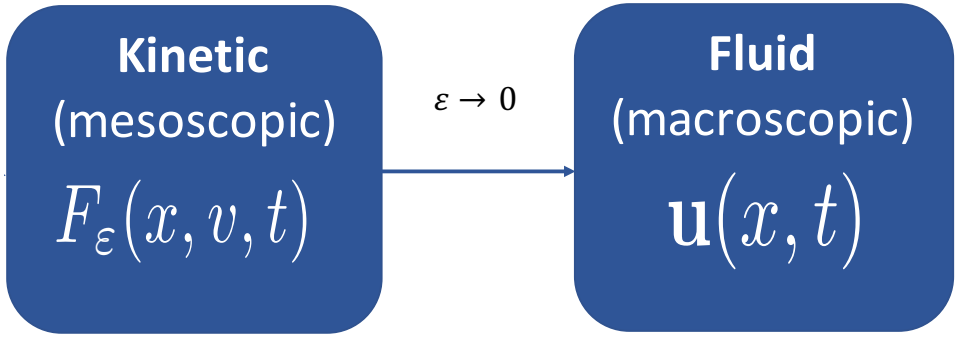
Challenges

$$\partial_t F_\varepsilon + v \cdot \nabla_x F_\varepsilon + a[F_\varepsilon] \cdot \nabla_v F_\varepsilon = \frac{1}{\varepsilon} \mathcal{C}[F_\varepsilon]$$



The difference in cost between a kinetic model and a fluid model is the discretization of v.

- Discretization in v is expensive, but easy to parallelize when $\varepsilon \gg 1$.
- Fluid approximations are cheap, but only accurate when $\varepsilon \ll 1$.
- Kinetic equations involve different types of operators.

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Toy model with linear algebra

- Start with a matrix equation for a vector $y \in \mathbb{R}^n$:

$$\boxed{Ay = \frac{1}{\varepsilon}(\overline{y}e - y) + q, \qquad A \in \mathbb{R}^{n\times n}, \quad q \in \mathbb{R}^n \quad e = (1, \ldots, 1) \in \mathbb{R}^n, \quad \overline{y} = \frac{1}{n}\sum_i y_i = \frac{1}{n}e^T y, \quad \varepsilon > 0}$$

- Assume
  1. $A + cI$ is "easy to invert" for any constant c
  2. $e^T A e = \sum_{i,j} A_{i,j} > 0$
- Average model for y:

$$\boxed{\overline{Ay} = \overline{q}}$$

- Closure: for ε small, $y = \overline{y}e + \mathcal{O}(\varepsilon)$. Thus

$$\boxed{\overline{y} = \frac{n\overline{q}}{e^T A e} + \mathcal{O}(\varepsilon)} \quad \Rightarrow \quad \boxed{y = \frac{n\overline{q}}{e^T A e}e + \mathcal{O}(\varepsilon)}$$

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Creating the hybrid

- The original system is

$$\boxed{Ay = \frac{1}{\varepsilon}(\overline{y}e - y) + q}$$

- Let $y = y_0 + y_1$, where

$$\boxed{\begin{aligned} Ay_0 &= -\frac{1}{\varepsilon}y_0 + q, \\ Ay_1 &= \frac{1}{\varepsilon}(\overline{y_1}e - y_1) + \frac{1}{\varepsilon}\overline{y_0} \end{aligned}}$$

- Hybrid idea: Use the reduced model to find $y_1^* \approx y_1$

$$\boxed{\begin{aligned} Ay_0 &= -\frac{1}{\varepsilon}y_0 + q, \\ \overline{y_1^*} &= \frac{1}{\varepsilon}\frac{n\overline{y_0}}{e^T Ae}, \quad y_1^* = \overline{y_1^*}e \end{aligned}} \quad \Rightarrow \quad \boxed{y \approx y^* = y_0 + y_1^*}$$

Linear kinetic model

- We want to solve the linear kinetic equation

$$\partial_t F + v \cdot \nabla_x F + a \cdot \nabla_v F = \frac{1}{\varepsilon} \underbrace{(\mathcal{S}F - F)}_{\mathcal{C}(F)} + q$$

  where the integral operator $\mathcal{S}$ is represents a weighted average, with implicit time steps.

- Collided/uncollided splitting: $F = F_0 + F_1$, where

$$\partial_t F_0 + v \cdot \nabla_x F_0 + a \cdot \nabla_v F_0 = -\frac{1}{\varepsilon} F_0 + q$$

$$\partial_t F_1 + v \cdot \nabla_x F_1 + a \cdot \nabla_v F_1 = \frac{1}{\varepsilon}(\mathcal{S}F_1 - F_1) + \frac{1}{\varepsilon}\mathcal{S}F_0$$

- Idea: Solve for F_0 with high resolution in v. Solve for F_1 with low resolution (i.e. a reduced model).

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Why is this a good idea?

- Works well for both collisionless ($\varepsilon \gg 1$) and highly-collisional regimes ($\varepsilon \ll 1$).
- Amenable to parallelization.
- Flexibility allows for different numerical treatments of F_0 and F_1, thereby improving efficiency.
- Correction tools can address errors due to splitting, nonlinearities, discretization.
- Finer splittings based on degree of "collisionality" ($F_0, F_1, \ldots, F_k$) are straight-forward.

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Where have we made progress?

- **Correction strategies that accounts for both hybrid and temporal error**
  - M. M. Crockatt, A. J. Christlieb, C. K. Garrett, and C. D. Hauck, *An arbitrary-order, fully implicit, hybrid kinetic solver for linear radiative transport using integral deferred correction*, Journal of Computational Physics, (2017)
  - M. M. Crockatt, A. J. Christlieb, C. K. Garrett, and C. D. Hauck, *Hybrid methods for radiation transport using diagonally implicit Runge-Kutta and space-time discontinuous Galerkin time integration*, Journal of Computational Physics, (submitted)
- **Fast iterative methods for acceleration in phase space**
  - C. K. Garrett and C. D. Hauck, *A fast solver for implicit integration of the Vlasov–Poisson system in the eulerian framework*, SIAM Journal on Scientific Computing, 40 (2018), pp. B483–B506
- **Dedicated operator discretizations for increased resolution**
  - G. Dimarco, C. D. Hauck, and R. R. Loubère, *A class of low dissipative schemes for solving kinetic equations*, Journal of Scientific Computing, (to appear)
- **Fast evaluation of collision operators**
  - I. M. Gamba, J. R. Haack, C. D. Hauck, and J. Hu, *A fast spectral method for the Boltzmann collision operator with general collision kernels*, SIAM Journal on Scientific Computing, 39 (2017), pp. B658–B674

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Where have we made progress?

- **Approximate collision models**
  - J. R. Haack, C. D. Hauck, and M. S. Murillo, *A conservative, entropic multispecies BGK model*, Journal of Statistical Physics, 168 (2017), pp. 826–856
  - ———, *Interfacial mixing in high-energy-density matter with a multiphysics kinetic model*, Physical Review E, 96 (2017), p. 063310
- **Rigorous multi-scale error analysis**
  - Z. Chen and C. D. Hauck, *Multiscale convergence properties for spectral approximations of a model kinetic equation*, Mathematics of Computation, (submitted)
- **Low-memory implementations based on hybridization in the spatial discretizations**
  - Z. Sun and C. D. Hauck, *A low memory discrete ordinates discontinuous Galerkin method for the radiative transport equation*, (in preparation)
  - C. D. Hauck, Q. Sheng, and Y. Xing, *An asymptotic preserving hybrid finite volume discontinuous Galerkin method for transport equations*, (in preparation)
- **Improved treatment of boundary conditions**
  - Z. Chen and C. D. Hauck, *Boundary corrections for hybrid methods*, (in preparation)
- **Extension to nonlinear problems in radiation, electron transport, and gas dynamics.**
  - Z. Chen, C. K. Garrett, C. D. Hauck, and M. P. Laiu, *An implicit hybrid solver for kinetic semiconductor equations*, (in preparation)

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Some examples

Simulation example: integral deferred correction

- **Background:** Integral deferred correction is a time integration technique that systematically lifts low-order methods to high-order by repetitive solution of an error equation.
- **Idea:** Use integral deferred correction to improve (1) temporal accuracy and (2) errors in the hybrid approximation.
- **Application:** The algorithm is applied to several test problem relevant to radiation transport.
- **Result:** Gains in efficiency allow for more resolution of fine scale features, thereby giving better answers is a fraction of the time.

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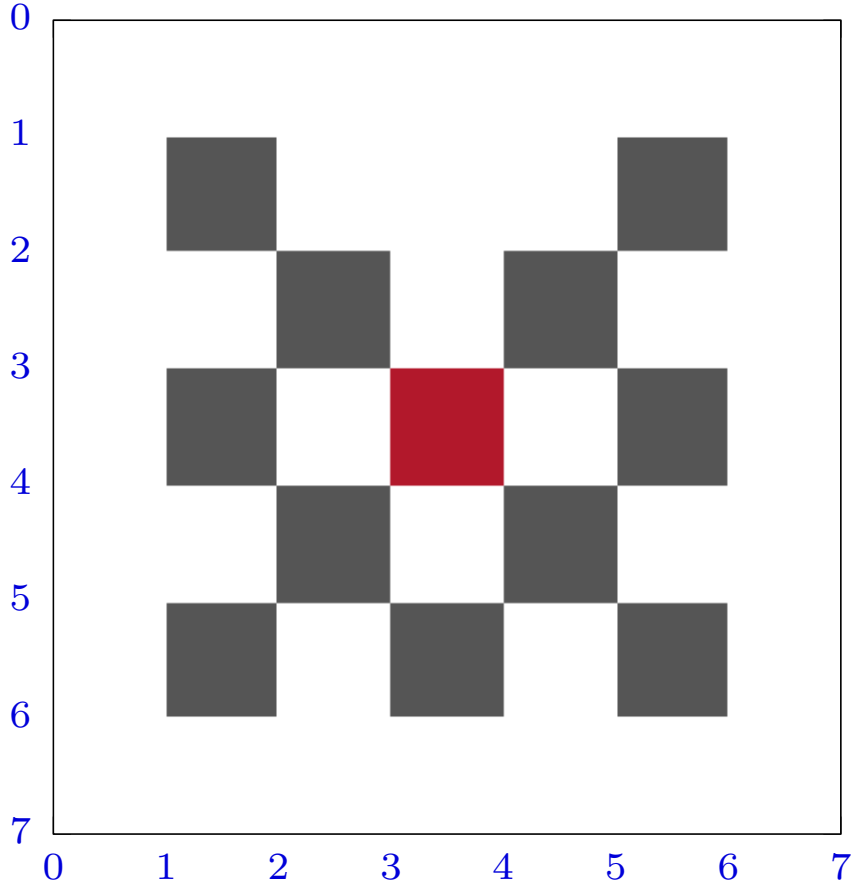
The 2D lattice test problem



Region	σ_t	σ_s	σ_a	Q
white	1	1	0	0
red	1	1	0	1
gray	10	0	10	0

Order:	5
IDC substeps:	3
IDC corrections:	4
Spatial cells:	168
Final time:	3.2
CFL:	25.6

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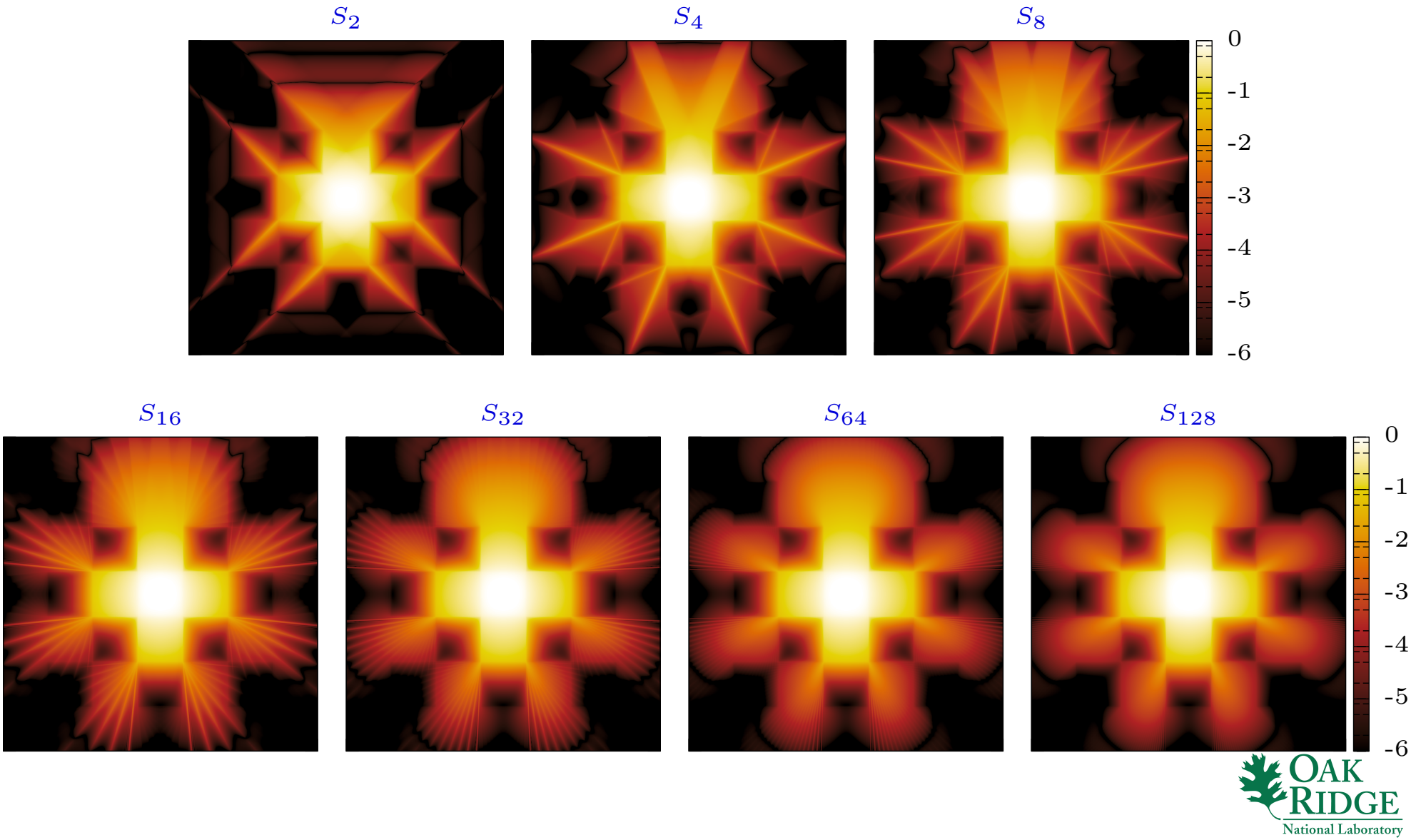
Solutions under refinement



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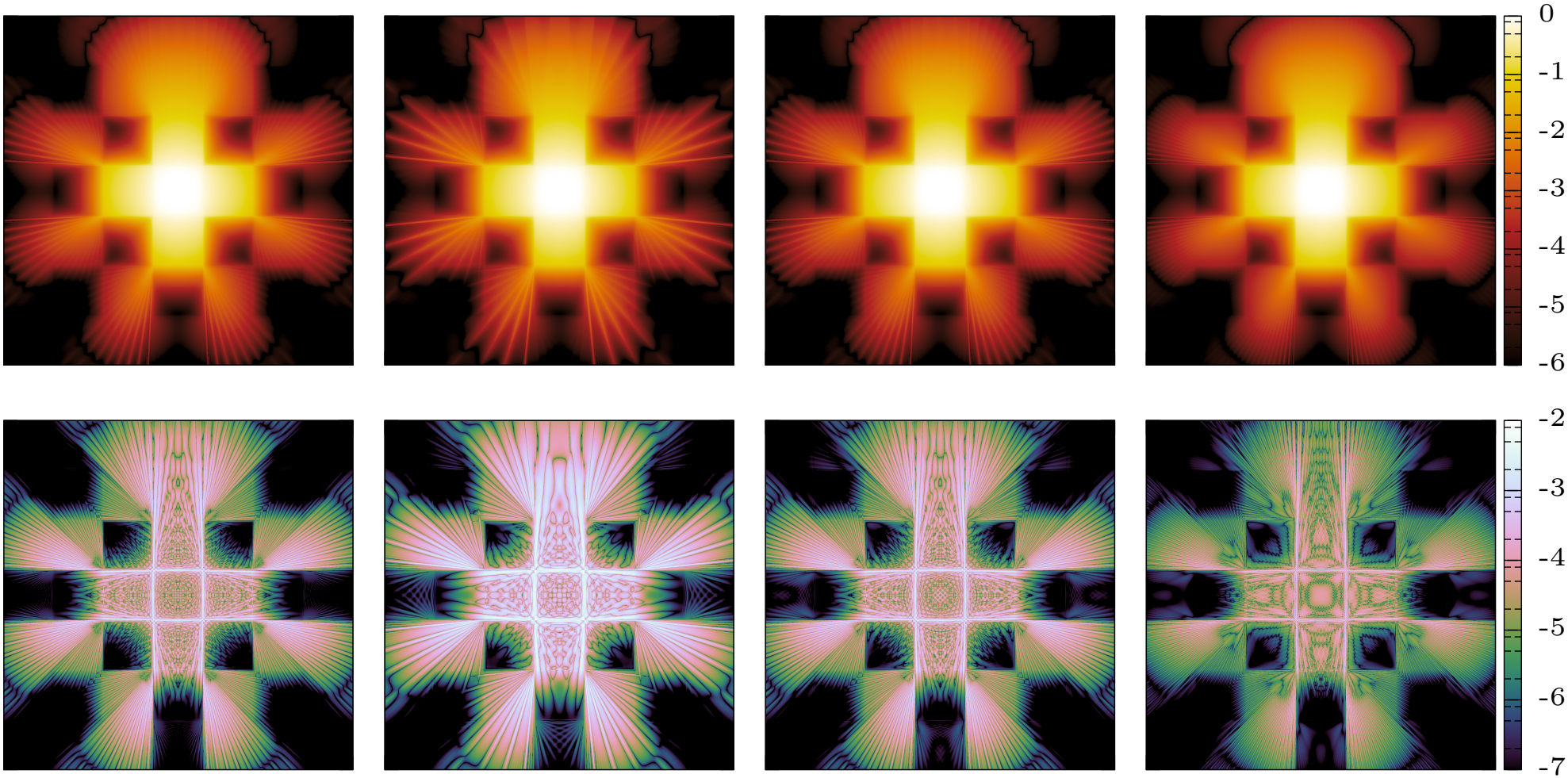
Hybrid solutions

S_{32} : 100%($\sim$ 1hr.) S_{16} : 24%($\sim$ 16min.) $S_{32\text{-}4}$: 16%($\sim$ 10min.) $S_{64\text{-}4}$: 59%($\sim$ 38min.)



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Modeling example: approximate collision operators

- **Background:** In gas dynamics, the (BGK) Bhatnagar–Gross–Krook collision operator is used to approximation the very expensive Boltzmann collision operator (5D integral).
- **Idea:** Extend the BGK operator to the multi-species setting, while maintaining important conservation and stability properties.
- **Application:** We apply the method to an interface problem that models ablator-fuel mixing in an inertial confinement fusion target.
- **Result:** The cost reduction enables exploration of scenarios over a wide range of energies. We demonstrate that (i) for moderate energy profiles, single fluid models are not sufficient and (ii) for high-energies, kinetic effects are important.

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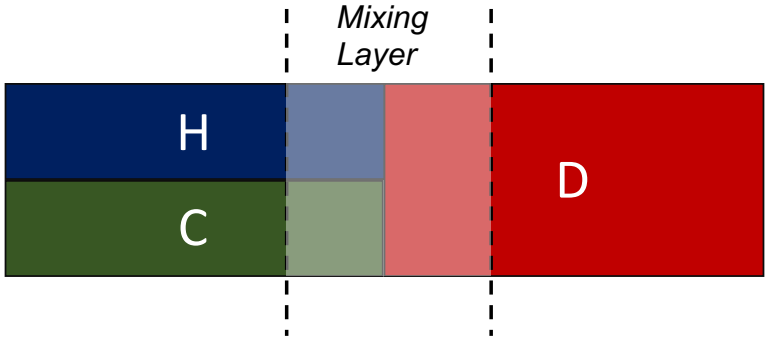
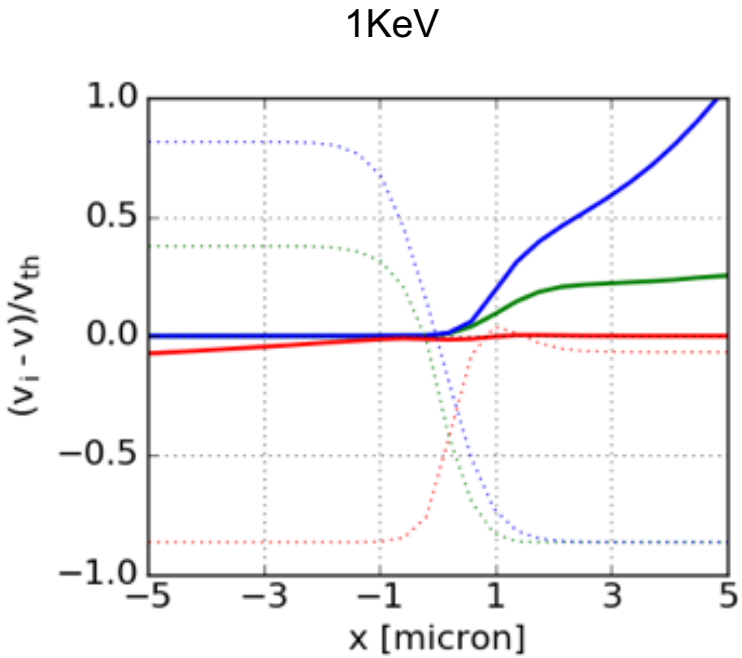
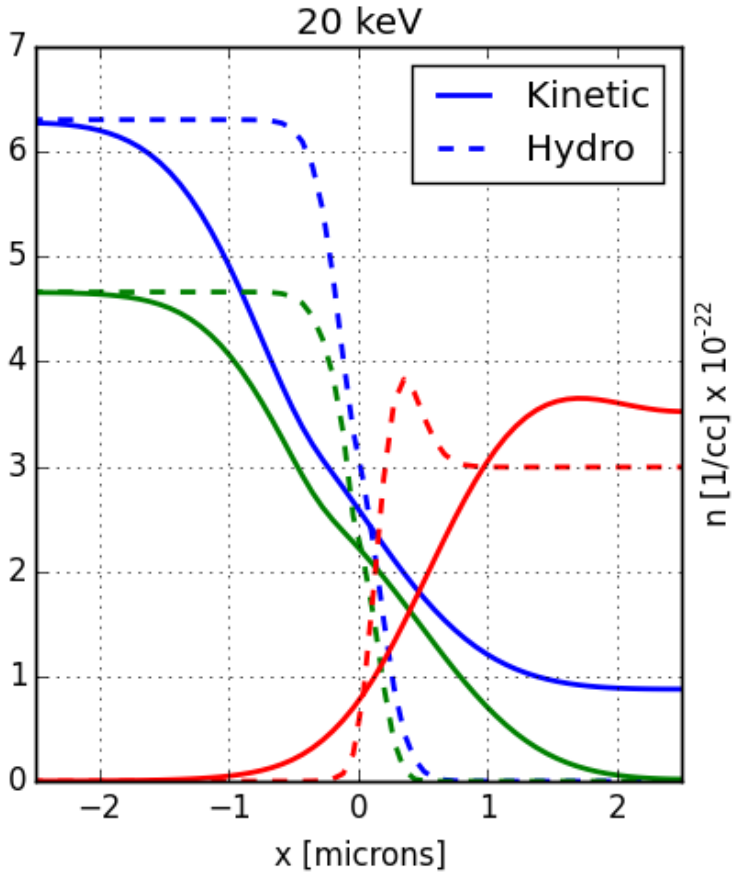
Simulation of a fuel-ablator interface







Analysis example: multi-scale error estimate

- **Background:** Kinetic equations can be approximated by
  1. fluid models with $\mathcal{O}(\varepsilon)$ error
  2. direct discretization of v with an $O(n^{-q})$ error; q smooothness, n unknowns.
- **Idea:** Prove ε-dependent estimates for the velocity discretization error when $0 \ll \varepsilon < 1$.
- **Application:** We consider a prototype linear kinetic equation with periodic boundaries.
- **Result:** Using a specially constructed energy functional, we derive error estimates that are (i) much sharper than standard approximation theory results and (ii) actually observed in practice.

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Multi-scale error estimate

Theorem

Suppose that $g_0 \in H^1(dx)$. *Then there exists an absolute constant* $\lambda_1 > 0$ *such that the* L^2 *error of the* P_n *approximation satisfies*

$$\|F - F^n\|_{L^2(dvdx)}(t) \leq \cancel{B(g)e^{-\frac{\lambda_1 t}{\epsilon^2}}} + \cancel{C(\partial_x g)\sqrt{t}e^{-\frac{\lambda_1 t}{\epsilon^2}}} + D(g,n,t)\epsilon^{n+1},$$

where $D(g,n,t)$ *is positive and bounded for any* $t > 0$ *and is decreasing exponentially in* t *for* t *sufficiently large. Moreover, the* L^2 *error for each coefficient satisfies*

$$\|F_\ell - F_\ell^n\|_{L^2(dx)}(t) \leq \begin{cases} \cancel{C(\partial_x g)\sqrt{t}e^{-\frac{\lambda_1 t}{\epsilon^2}}} + E(g,n,2,t)\epsilon^{2n}, & \ell = 0, \\ \cancel{C(\partial_x g)\sqrt{t}e^{-\frac{\lambda_1 t}{\epsilon^2}}} + E(g,n,\ell,t)\epsilon^{2n+2-\ell}, & 1 \leq \ell \leq n, \end{cases}$$

where $E(g,n,\ell,t)$ *is positive and bounded for any* $t > 0$ *and is monotonically decreasing with respect to* t.

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Technical Outlook

- After some initial ramp up period, development of the hybrid kinetic strategy is progressing nicely
- Major things to do:
  - Nonlinear problems
  - More error estimation
  - Adaptivity
- Acceleration of molecular dynamics simulations is lurking in the future.

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Practical Challenges

- **Impact:**
  - What is the work flow to reach an "end product"?
  - What is my role in that work flow?
- **Stability:**
  - What is the best way to create a sustainable effort?

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Thank You!

References

Z. Chen, C. K. Garrett, C. D. Hauck, and M. P. Laiu, *An implicit hybrid solver for kinetic semiconductor equations*, (in preparation).

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