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MODELS & MEASURES OF MIXING & EFFECTIVE DIFFUSION

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***Big questions*:**

How can we gauge the effectiveness of a stirrer as a mixer?

How might we parameterize stirring as diffusion?

***Outline*:**

- Models
- Conflicts
- Resolution
- More models
- Reconciliation

Mathematical models of mixing

Given flow field $\vec{u}(\vec{x},t)$ with $\nabla \cdot \vec{u} = 0$, consider

Stochastic Diff Eq: $d\vec{X}(t) = \vec{u}(\vec{X},t)dt + \sqrt{2\kappa}\, d\vec{W}(t)$

- $\boldsymbol{X}(t)$ is passive tracer particle position
- κ is the molecular diffusion coefficient

Advection - Diffusion Eq: $\partial_t \theta + \vec{u} \cdot \nabla \theta = \kappa \Delta \theta + s$

- $\theta(\boldsymbol{x},t)$ is passive scalar density, concentration
- $s(\boldsymbol{x},t)$ is passive scalar source-sink distribution
- plus appropriate initial and boundary conditions

Mathematical measures of mixing

Temptation & tradition suggest characterizing stirring as an "effective" diffusion

$$\vec{u} \cdot \nabla - \kappa \Delta \;\rightarrow\; -\partial_i K_{ij}^{eff} \partial_j$$

Three questions:

- Which aspects of mixing should be encoded in $\boldsymbol{K}^{eff}$?
- Do different criteria produce different $\boldsymbol{K}^{eff}$?
- Transferable among applications?

Mathematical measures of mixing

$$\text{Measure 1: } K^{PD} = K_{ij}^{eff}$$

$$\text{Measure 2: } K^{FG} = K_{11}^{eff}$$

$$\text{Measure 3: } \kappa_p^{VR} = \kappa_p^{eff} \quad \text{for } p = +1, 0, -1$$

$p = +1, 0, -1$ ~ "small", "intermediate", or "large" scale variance reduction

Mathematical measures of mixing

$$\text{Measure 1: } K^{PD} = K_{ij}^{eff}$$

via tracer particle dispersion

$$\mathbf{E}\left\{\left(X_i(t) - X_i(0)\right)\left(X_j(t) - X_j(0)\right)\right\} \sim 2K_{ij}^{eff}\, t$$

as $t \to \infty$.

Mathematical measures of mixing

$$\text{Measure 2}: \; K^{FG} = K_{11}^{eff}$$

$$\text{via flux-gradient relation}, \;\; T = -Gx + \theta \;\Rightarrow$$

$$\partial_t \theta + \vec{u} \cdot \nabla \theta = \kappa \Delta \theta + G\left(\hat{i} \cdot \vec{u}\right)$$

$$\text{everything mean zero \& periodic on a cell} \;\; \Rightarrow$$

$$K_{11}^{eff} = \kappa + \frac{\left\langle u_1 \theta \right\rangle}{G} = \kappa \left(1 + \frac{\left\langle |\vec{\nabla} \theta|^2 \right\rangle}{G^2} \right)$$

Mathematical measures of mixing

$$\text{Measure 3: } \kappa_0^{VR} = \kappa^{eff}$$

via concentration variance reduction

For $s(\vec{x})$ mean 0 and $\partial_t \theta + \vec{u} \cdot \nabla \theta = \kappa \Delta \theta + s(\vec{x})$

$$\kappa^{eff} = \sqrt{\frac{\left\langle \left(\Delta^{-1} s \right)^2 \right\rangle}{\left\langle \theta^2 \right\rangle}}$$

Mathematical measures of mixing

Multiscale Measure 3(a): $\kappa_p^{VR} = \kappa_p^{eff}$

via concentration (*inverse*) *gradient* variance reduction

For $s(\vec{x})$ mean 0 and $\partial_t \theta + \vec{u} \cdot \nabla \theta = \kappa \Delta \theta + s(\vec{x})$

$$\kappa_{\pm 1}^{eff} = \sqrt{\frac{\left\langle \left| \nabla^{\pm 1} \Delta^{-1} s \right|^2 \right\rangle}{\left\langle \left| \nabla^{\pm 1} \theta \right|^2 \right\rangle}}$$

Mathematical measures of mixing

$$\text{Measure 1}: \; K^{PD} = K_{ij}^{eff} \sim \frac{1}{2t} \mathbf{E}\left\{ \left(X_i(t) - X_i(0) \right) \left(X_j(t) - X_j(0) \right) \right\}$$

$$\text{Measure 2}: \; K^{FG} = K_{11}^{eff} = \kappa \left(1 + \frac{\left\langle |\vec{\nabla}\theta|^2 \right\rangle}{G^2} \right)$$

$$\text{Measure 3}: \; \kappa_p^{VR} = \kappa_p^{eff} = \sqrt{\frac{\left\langle \left| \nabla^p \Delta^{-1} s \right|^2 \right\rangle}{\left\langle \left| \nabla^p \theta \right|^2 \right\rangle}} \; \text{ for } \; p = +1, 0, -1$$

Strength of stirring

Dimensionless ***Péclet*** number : $\quad \mathrm{Pe} \equiv \frac{U\ell}{\kappa}$

$U \sim$ velocity scale ... $\ell \sim$ length scale

Dimensionless ***Enhancement*** or ***Efficacy*** factor:

$$E(\mathrm{Pe}) \equiv \frac{\kappa_p^{VR}}{\kappa} \text{ or } \frac{K^{PD,FG}}{\kappa}$$

Fact:

In terms of tracer dispersion or flux-gradient relation, there are flows for which the enhancement may be as large as

$$E(\mathrm{Pe}) = \frac{K^{FG}}{\kappa} \sim \mathrm{Pe}^2 \quad \text{as} \quad \mathrm{Pe} \to \infty.$$

Fact:

In terms of concentration variance reduction in presence of steady sources & sinks the enhancement cannot be that big.

$$\textbf{\textit{Theorem}}: \quad E(\mathrm{Pe}) = \frac{\kappa_p^{VR}}{\kappa} \le \mathrm{Pe}^1 \quad \text{as} \quad \mathrm{Pe} \to \infty.$$

CONFLICT !

Resolution

- What length scale ℓ is used in Pe = $U\ell/\kappa$?

In examples where $\dfrac{K^{FG}}{\kappa} \sim \mathrm{Pe}^2$ as $\mathrm{Pe} \to \infty$,

$$\mathrm{Pe} \equiv \frac{U\ell_{flow}}{\kappa}.$$

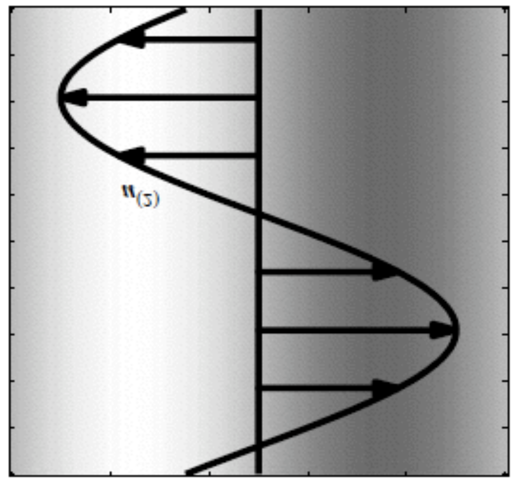
In theorem where $E(\mathrm{Pe}) = \dfrac{\kappa_p^{VR}}{\kappa} \leq \mathrm{Pe}^1$ as $\mathrm{Pe} \to \infty$,

$$\mathrm{Pe} \equiv \frac{U\ell_{source}}{\kappa} = \left(\frac{\ell_{source}}{\ell_{flow}}\right) \times \frac{U\ell_{flow}}{\kappa}.$$

Example: Basic Two-scale Model

A single-scale flow stirring a single-scale source-sink distribution

$$\vec{u}(\vec{x}) = \hat{i}\,\sqrt{2}\,U\,\sin k_u y$$



$$s(\vec{x}) = \sqrt{2}\,S\,\sin k_s x$$

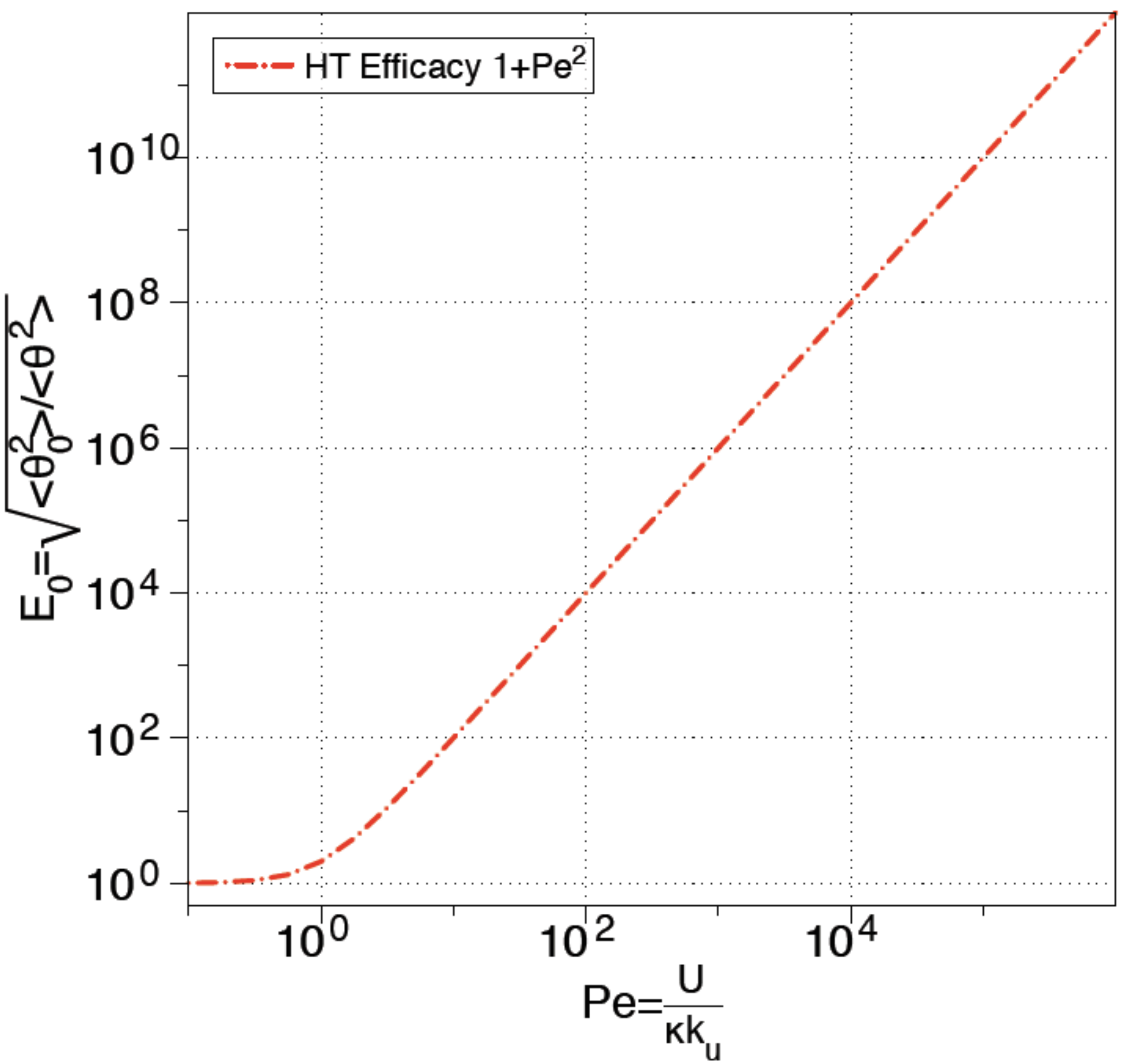
Two parameters: $\mathrm{Pe} \equiv \dfrac{U}{\kappa k_u}$ and $r = \dfrac{\ell_{source}}{\ell_{flow}} = \dfrac{k_u}{k_s}$

Dispersion/Flux-gradient mixing measure

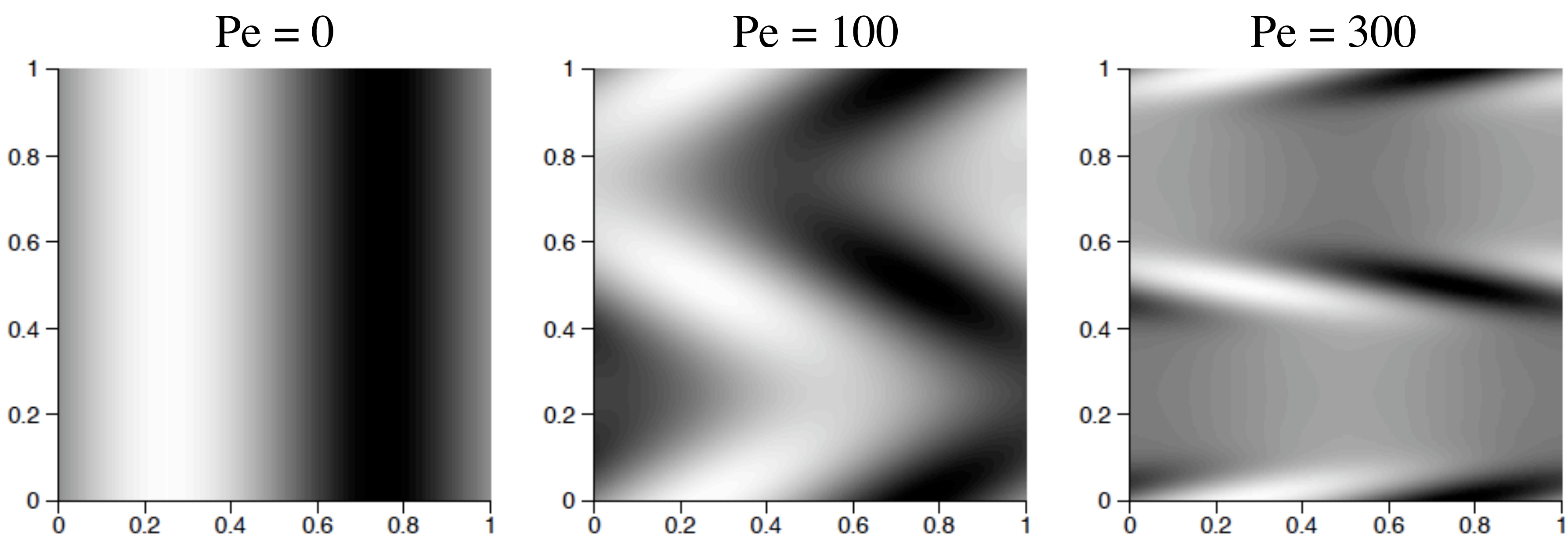
- a.k.a. **Homogenization Theory** (HT) …
- … presumably good for $\boldsymbol{r = k_u/k_s >> 1}$:
- $\dfrac{K^{FG}}{\kappa} = 1+\mathrm{Pe}^2 \quad \Rightarrow \quad$ HT approximation is

$$0 = K^{FG}\frac{d^2\theta_{\mathrm{HT}}(x)}{dx^2} + s(x) \quad \Rightarrow \quad \theta_{\mathrm{HT}}(x) = \frac{\sqrt{2}\,S\sin k_s x}{\kappa k_u^2(1+\mathrm{Pe}^2)}$$

$$\text{HT appx of } \kappa_p^{VR} = \sqrt{\frac{\left\langle\left(\Delta^{-1}s\right)^2\right\rangle}{\left\langle\theta_{\mathrm{HT}}^2\right\rangle}} = \sqrt{\frac{\left\langle\left|\nabla^{\pm1}\Delta^{-1}s\right|^2\right\rangle}{\left\langle\left|\nabla^{\pm1}\theta_{\mathrm{HT}}\right|^2\right\rangle}} = \kappa(1+\mathrm{Pe}^2)$$


HT Efficacy 1+Pe^2
10^10
10^8
10^6
10^4
10^2
10^0
10^0
10^2
10^4
E_0=√(<θ_0^2>/<θ^2>)
Pe=U/(κk_u)

Exact solution (for $r = 1$)

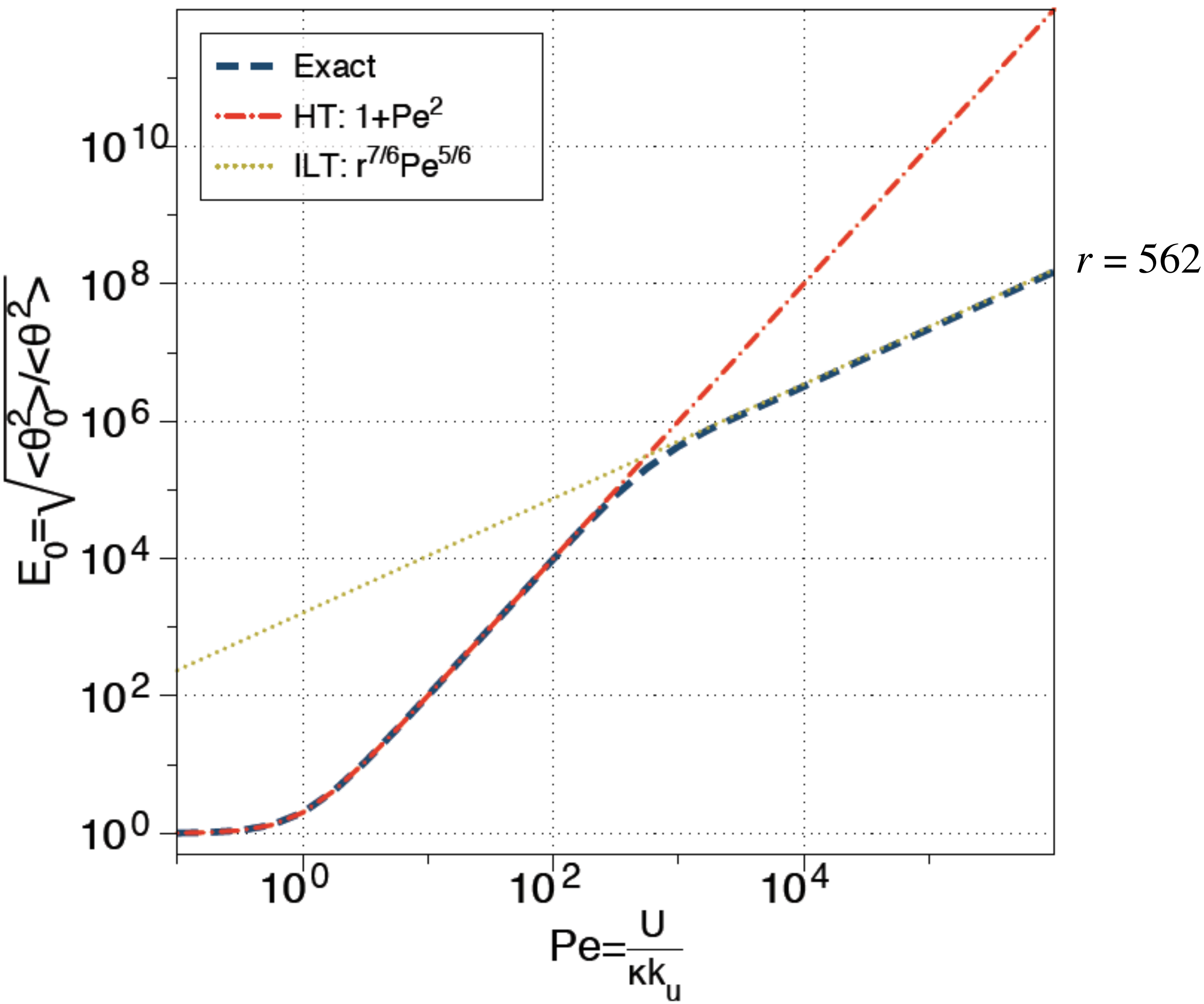


High-Pe (fixed r) asymptotic analysis: ***Internal-layer theory*** (ILT)

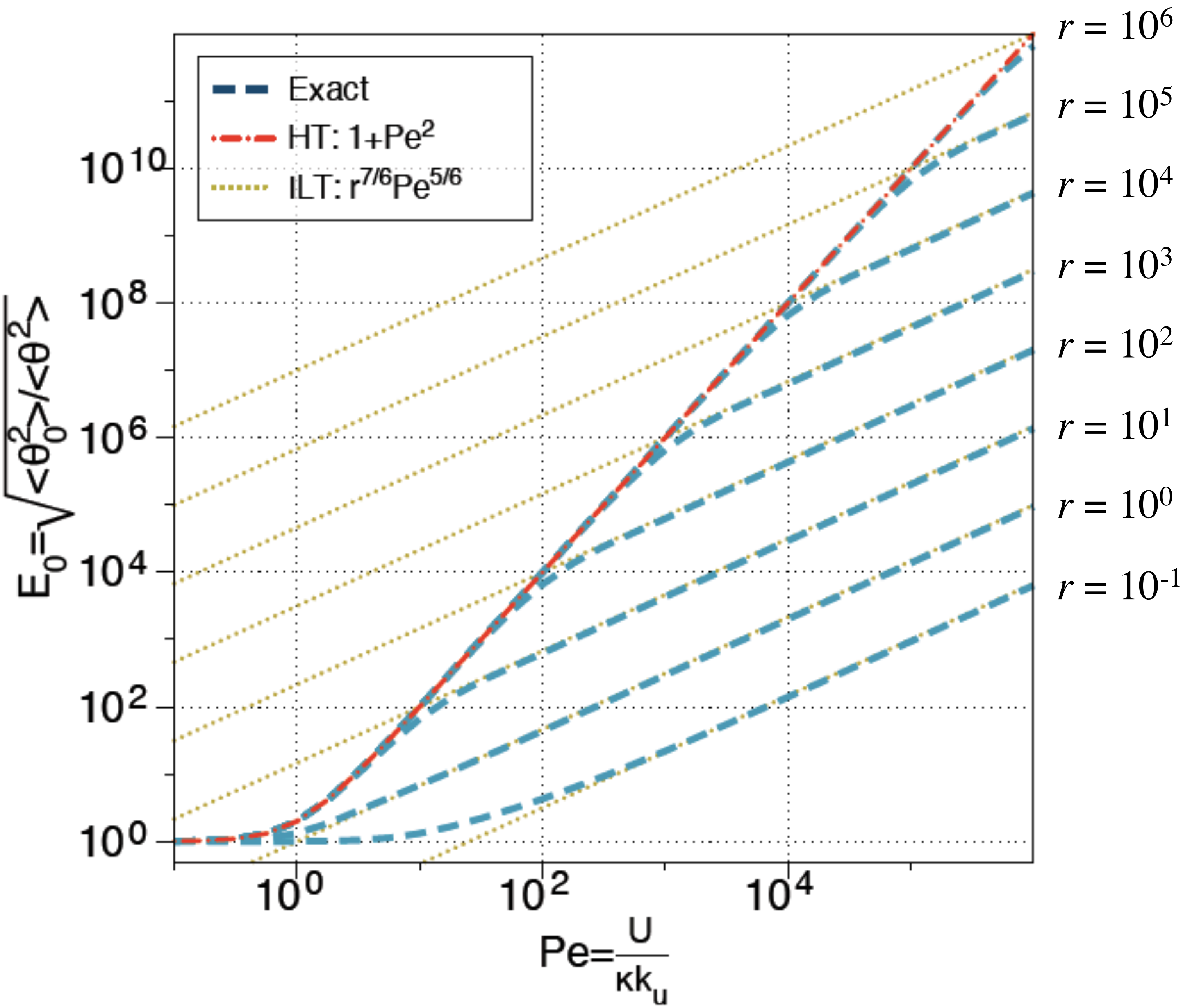
$$E_0 = \kappa_0^{VR}/\kappa \sim r^{7/6}\,\mathrm{Pe}^{5/6}$$

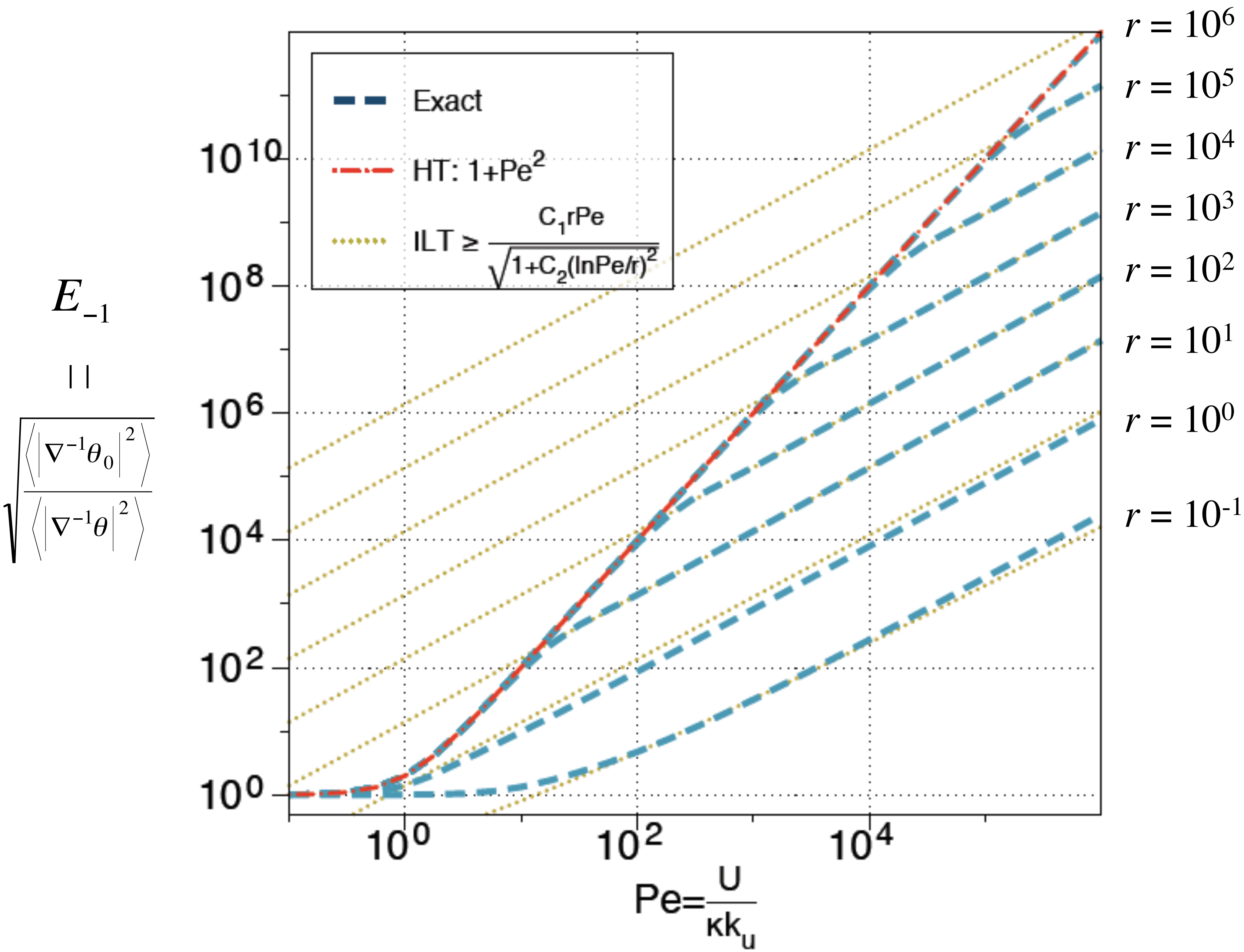
$$E_{+1} = \kappa_{+1}^{VR}/\kappa \sim r^{1/2}\,\mathrm{Pe}^{1/2}$$

$$E_{-1} = \kappa_{-1}^{VR}/\kappa \sim r\,\mathrm{Pe}$$

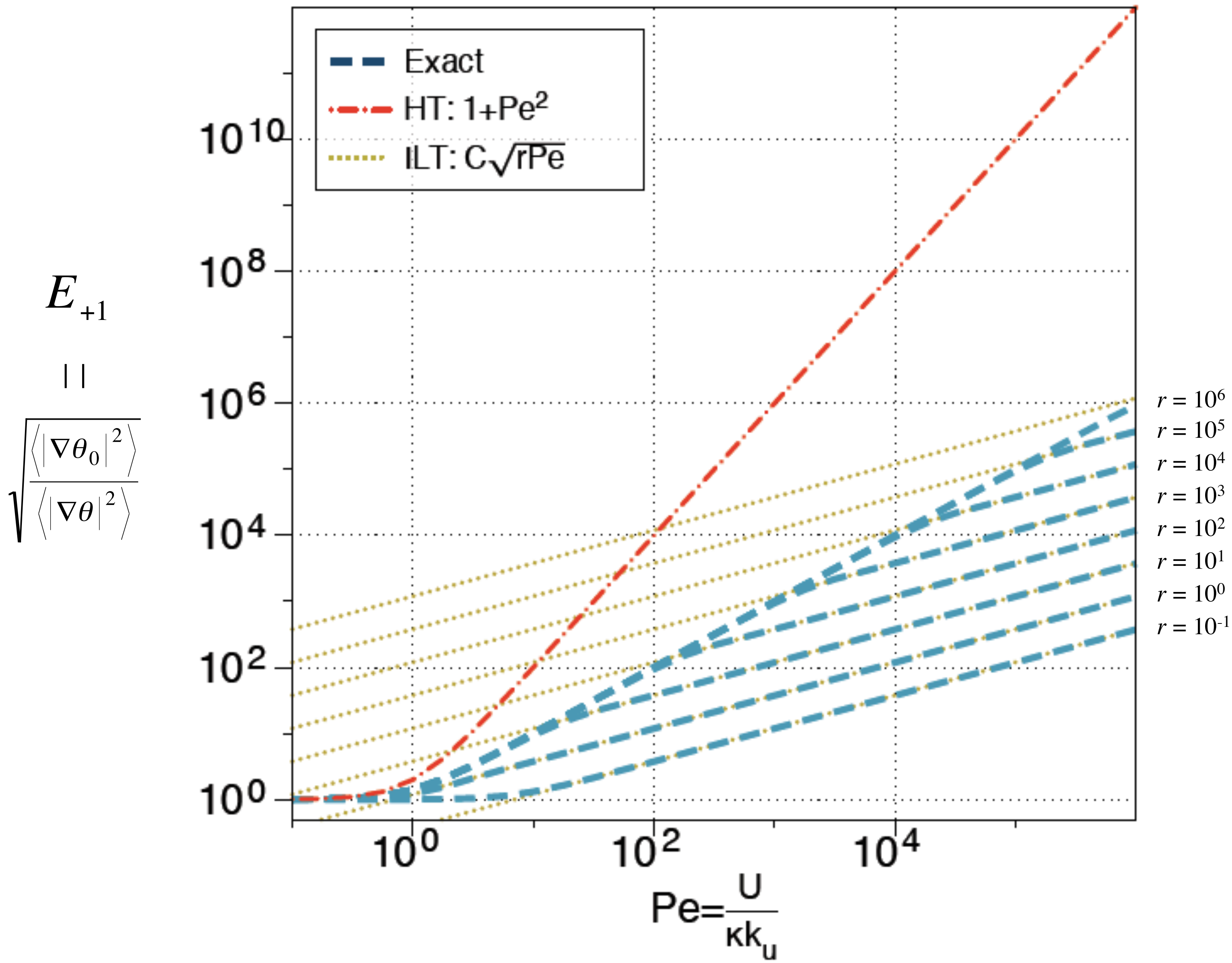


Exact
HT: 1+Pe^2
ILT: r^7/6Pe^5/6
10^10
10^8
10^6
10^4
10^2
10^0
E_0=√(<θ_0^2>/<θ^2>)
10^0
10^2
10^4
Pe=U/κk_u
r = 562


Exact
HT: 1+Pe^2
ILT: r$^{7/6}$Pe$^{5/6}$
10^{10}
10^8
10^6
10^4
10^2
10^0
$E_0=\sqrt{<\theta_0^2>/<\theta^2>}$
10^0
10^2
10^4
$Pe=\frac{U}{\kappa k_u}$
$r = 10^6$
$r = 10^5$
$r = 10^4$
$r = 10^3$
$r = 10^2$
$r = 10^1$
$r = 10^0$
$r = 10^{-1}$

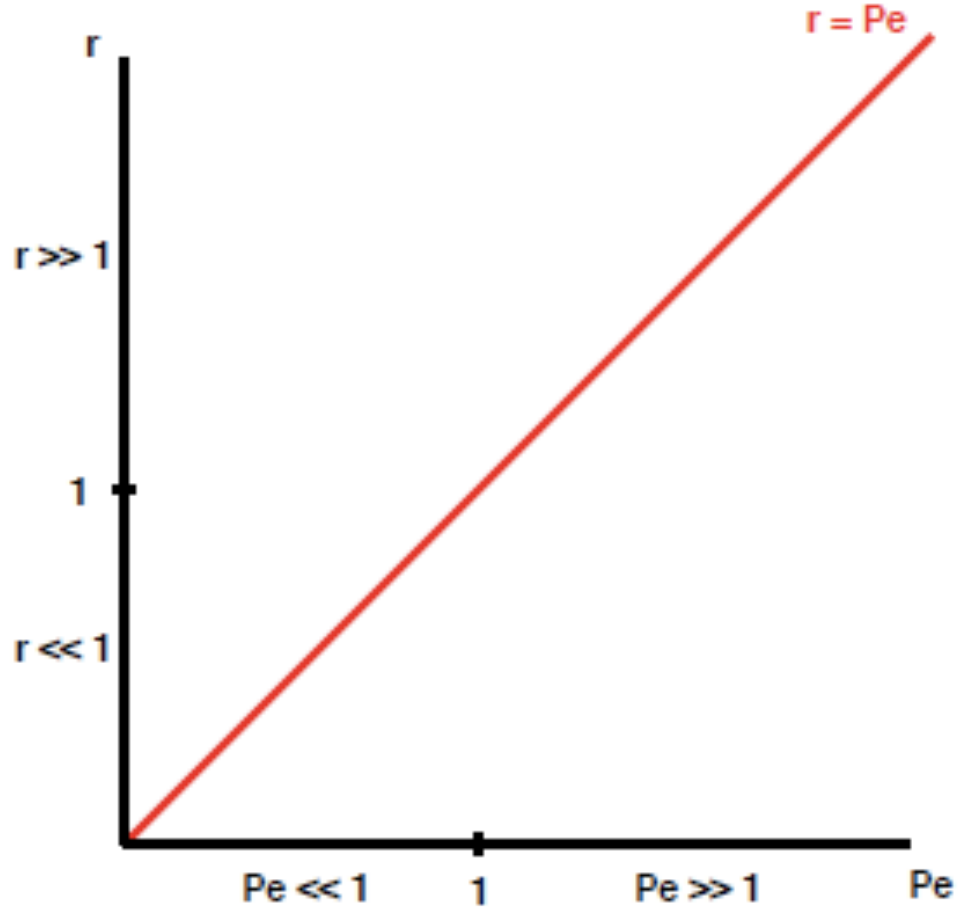


Exact
HT: 1+Pe^2
ILT ≥ $\frac{C_1 r Pe}{\sqrt{1+C_2(\ln Pe/r)^2}}$
$r = 10^6$
$r = 10^5$
$r = 10^4$
$r = 10^3$
$r = 10^2$
$r = 10^1$
$r = 10^0$
$r = 10^{-1}$
10^{10}
10^8
10^6
10^4
10^2
10^0
10^0
10^2
10^4
$E_{-1} = \sqrt{\frac{\langle|\nabla^{-1}\theta_0|^2\rangle}{\langle|\nabla^{-1}\theta|^2\rangle}}$
$Pe = \frac{U}{\kappa k_u}$

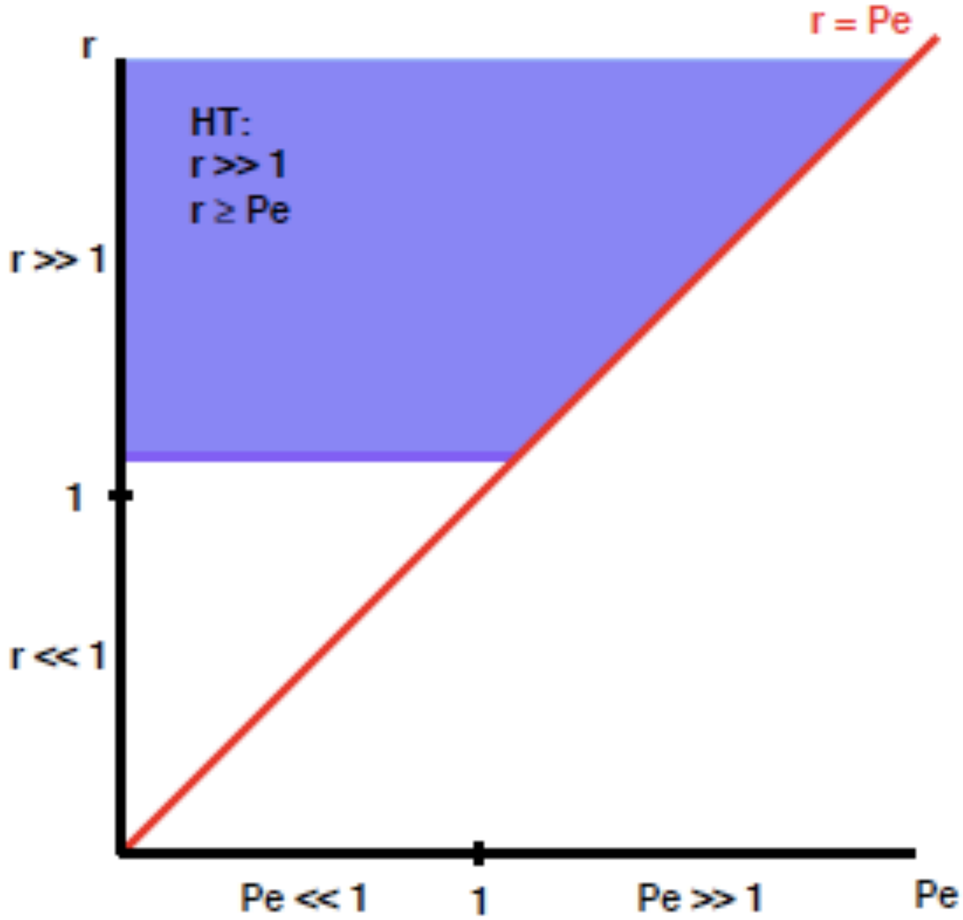


Exact
HT: 1+Pe²
ILT: C√rPe
10¹⁰
10⁸
10⁶
10⁴
10²
10⁰
10⁰
10²
10⁴
Pe=U/κk_u
E_+1
||
√(⟨|∇θ₀|²⟩/⟨|∇θ|²⟩)
r = 10⁶
r = 10⁵
r = 10⁴
r = 10³
r = 10²
r = 10¹
r = 10⁰
r = 10⁻¹

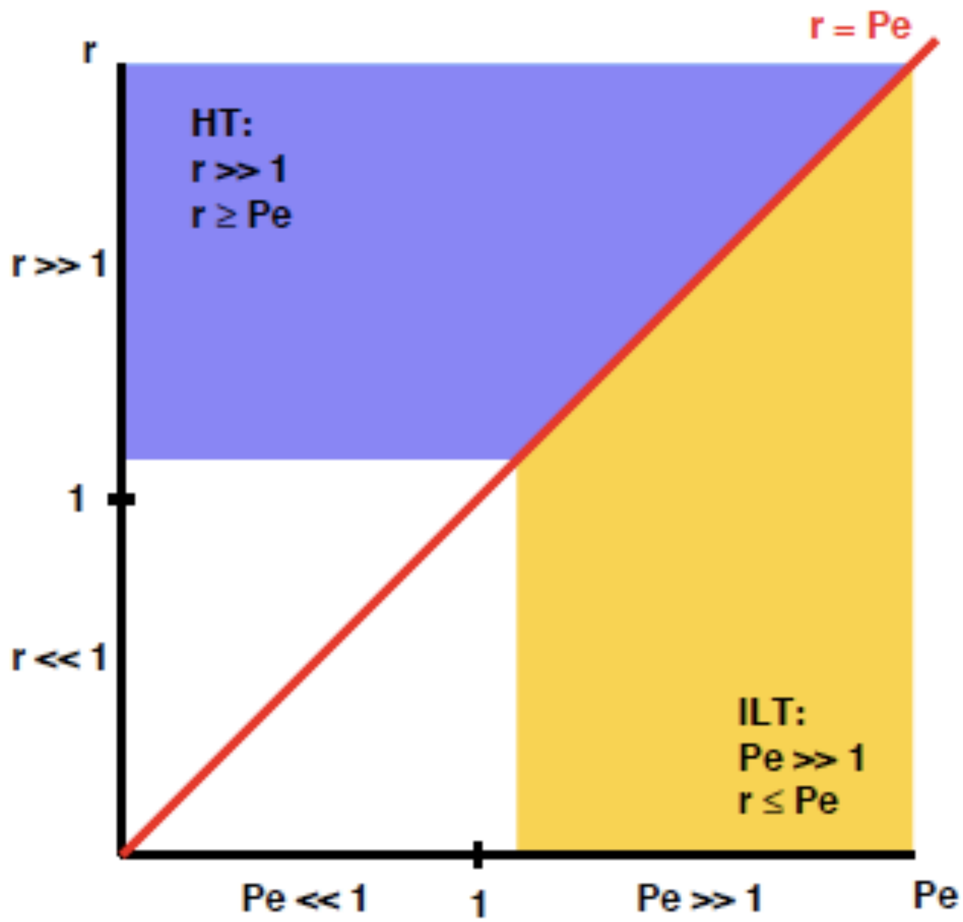
Stirring strength–scale separation phase diagram



Stirring strength–scale separation phase diagram



Stirring strength–scale separation phase diagram



Outline

- Models
- Conflicts
- Resolution
- More models
- Reconciliation

Questions:

- HT fails to predict the scalar variance sustained by steady sources & sinks when $\mathrm{Pe} > r >> 1$. Why?

- Can information about particle dispersion predict variance supression at high Péclet numbers?

- Particle dispersion is time and initial-location dependent …

$$\mathbf{E}\left\{\left(X_i(t)-X_i(0)\right)\left(X_j(t)-X_j(0)\right)\right\} \sim 2K_{i,j}^{PD}t$$

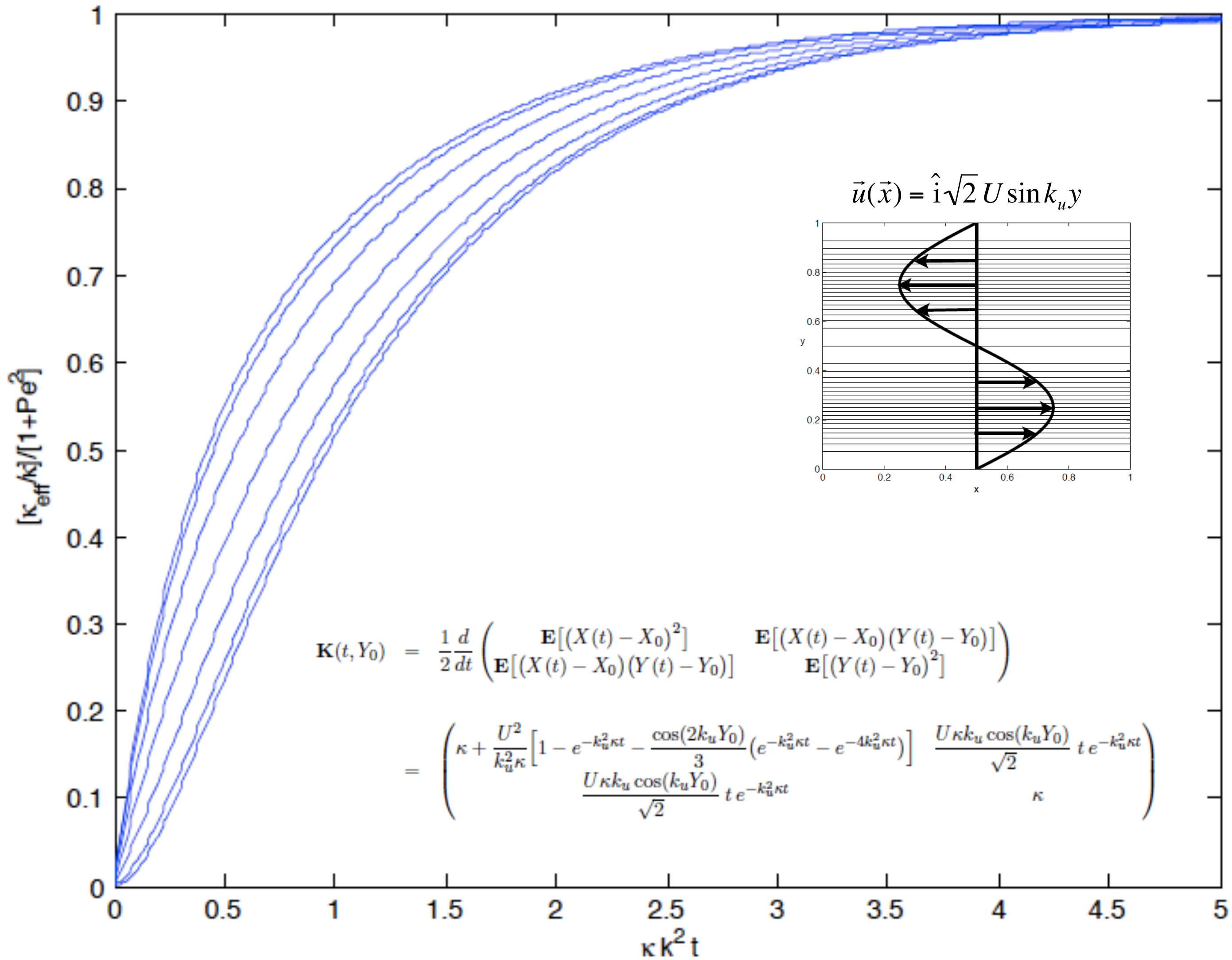
$$\Updownarrow$$

$$K_{i,j}^{PD}(t;\vec{X}(0)) \equiv \frac{d}{dt}\tfrac{1}{2}\mathbf{E}\left\{\left(X_i(t)-X_i(0)\right)\left(X_j(t)-X_j(0)\right)\right\}$$

- $\boldsymbol{K}^{\mathrm{PD}} \sim \kappa \mathrm{Pe}^2 = \mathcal{O}(\kappa^{-1})$ takes $\mathcal{O}(\ell_{flow}{}^2/\kappa)$ time to develop

... but $K_{i,j}^{PD}(t;\vec{X}(0)) \sim \kappa + U^2 t$ (at most) for $t \ll \ell_{flow}^2 / \kappa$.

Effective diffusion $K_{11}^{\mathrm{PD}}(t,y_0)$ vs. time



More modeling

- Concentration variance for stirred scalars sustained by inhomogeneous sources and sinks is dominated by the "latest" stuff introduced or deleted from the system.

- "Old" particles are relatively well mixed and so don't contribute substantially to the observed variance.

- Variance supression is controlled by particle dispersion rate on relatively ***short***, rather than ***long***, time scales at high Pe.

- In the presence of sustainted sources & sinks, even as $t \to \infty$ we cannot neglect transient behavior of $\boldsymbol{K}^{\mathrm{PD}}$ …

Dispersion-diffusion theory (DDT)

Given a stirring flow $\boldsymbol{u}(\boldsymbol{x},t)$ and its associated $\mathbf{K}_{ij}^{PD}$ $(t\text{-}t_0 | \boldsymbol{x}_0, t_0)$,

density due to stuff injected at $\boldsymbol{x}_0$, t_0 may best be described by

$$\partial_t \rho(\vec{x},t \mid \vec{x}_0,t_0) = \partial_i K_{ij}^{PD}(t - t_0 \mid \vec{x}_0,t_0)\partial_j \rho$$

$$\lim_{t \downarrow t_0} \rho(\vec{x},t \mid \vec{x}_0,t_0) = \delta(\vec{x},t \mid \vec{x}_0)$$

G. K. Batchelor, *Diffusion in a field of homogeneous turbulence I. Eulerian analysis*, Aust. J. Sci. Res. Series A, Phys. Sci., **2** (1949), 437–450.

Then the total density in presence of sources and sinks is ***at best*** described by

$$\theta_{\mathrm{DDT}}(\vec{x},t) = \int_{-\infty}^{t} dt_0 \int d\vec{x}_0 \rho(\vec{x},t \mid \vec{x}_0,t_0) s(\vec{x}_0,t_0)$$

… which does ***not*** satisfy an inhomogeneous diffusion equation!

On a periodic domain $[0,L]^d$

$$\rho(\vec{x},t \mid \vec{x}_0,t_0) = \frac{1}{L^d}\sum_{\vec{k}} \exp\left\{ i\vec{k}\cdot(\vec{x}-\vec{x}_0) - k_i k_j \int_{t_0}^{t} K_{ij}^{PD}(t'-t_0 \mid \vec{x}_0,t_0)dt' \right\}$$

$$\text{Note: } \boldsymbol{if} \quad K_{ij}^{PD} \sim \left[\kappa + U^2(t-t_0)\right]\delta_{ij} \text{ as } \quad t-t_0 \to 0, \ \boldsymbol{then}$$

$$\theta_{\mathrm{DDT}}(\vec{x},t) = \int_{-\infty}^{t} dt_0 \int d\vec{x}_0 \rho(\vec{x},t \mid \vec{x}_0,t_0)s(\vec{x}_0)$$

$$\Downarrow$$

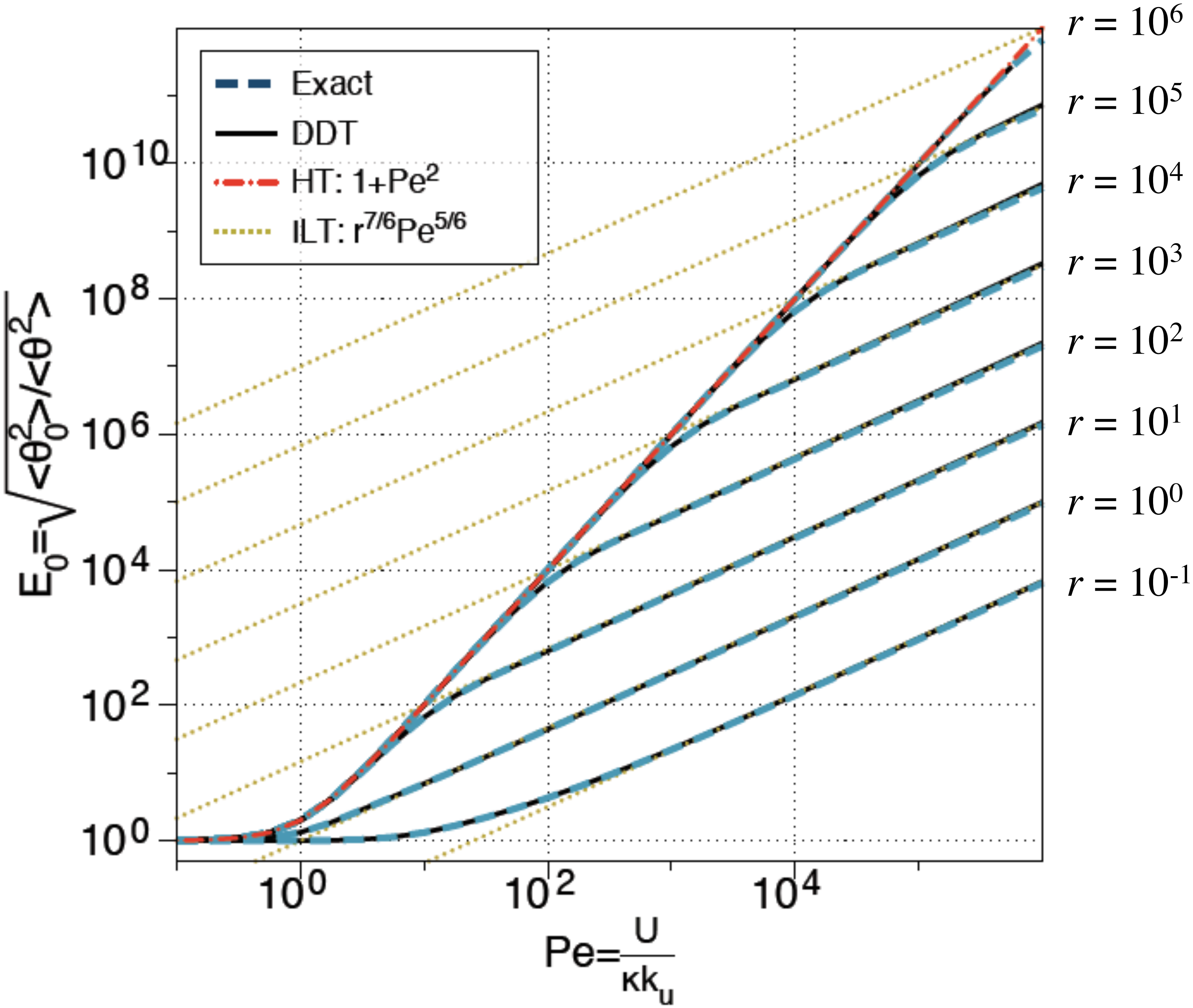
$$\hat{\theta}_{\mathrm{DDT}}(\vec{k}) \sim \hat{s}(\vec{k})\int_0^{\infty} e^{-\kappa k^2\tau - \frac{1}{2}k^2U^2\tau^2}\, d\boldsymbol{\tau}$$

$$\Rightarrow \text{ as } \mathrm{Pe} \to \infty, \quad \hat{\theta}_{\mathrm{DDT}}(\vec{k}) \sim \frac{\hat{s}(\vec{k})}{kU} \quad \text{so} \quad \kappa_0^{VR} = \sqrt{\frac{\left\langle \left(\Delta^{-1}s\right)^2 \right\rangle}{\left\langle \theta_{\mathrm{DDT}}^2 \right\rangle}} \sim U\ell_{source}$$

Reconciliation

- **$64** question: Is DDT quantitatively accurate?

- For single-scale flow stirring single-scale source …



Exact
DDT
HT: 1+Pe^2
ILT: r^{7/6}Pe^{5/6}
E_0=√(<θ_0^2>/<θ^2>)
Pe=U/(κk_u)
10^0
10^2
10^4
10^6
10^8
10^10
r = 10^6
r = 10^5
r = 10^4
r = 10^3
r = 10^2
r = 10^1
r = 10^0
r = 10^-1

More reconciliation

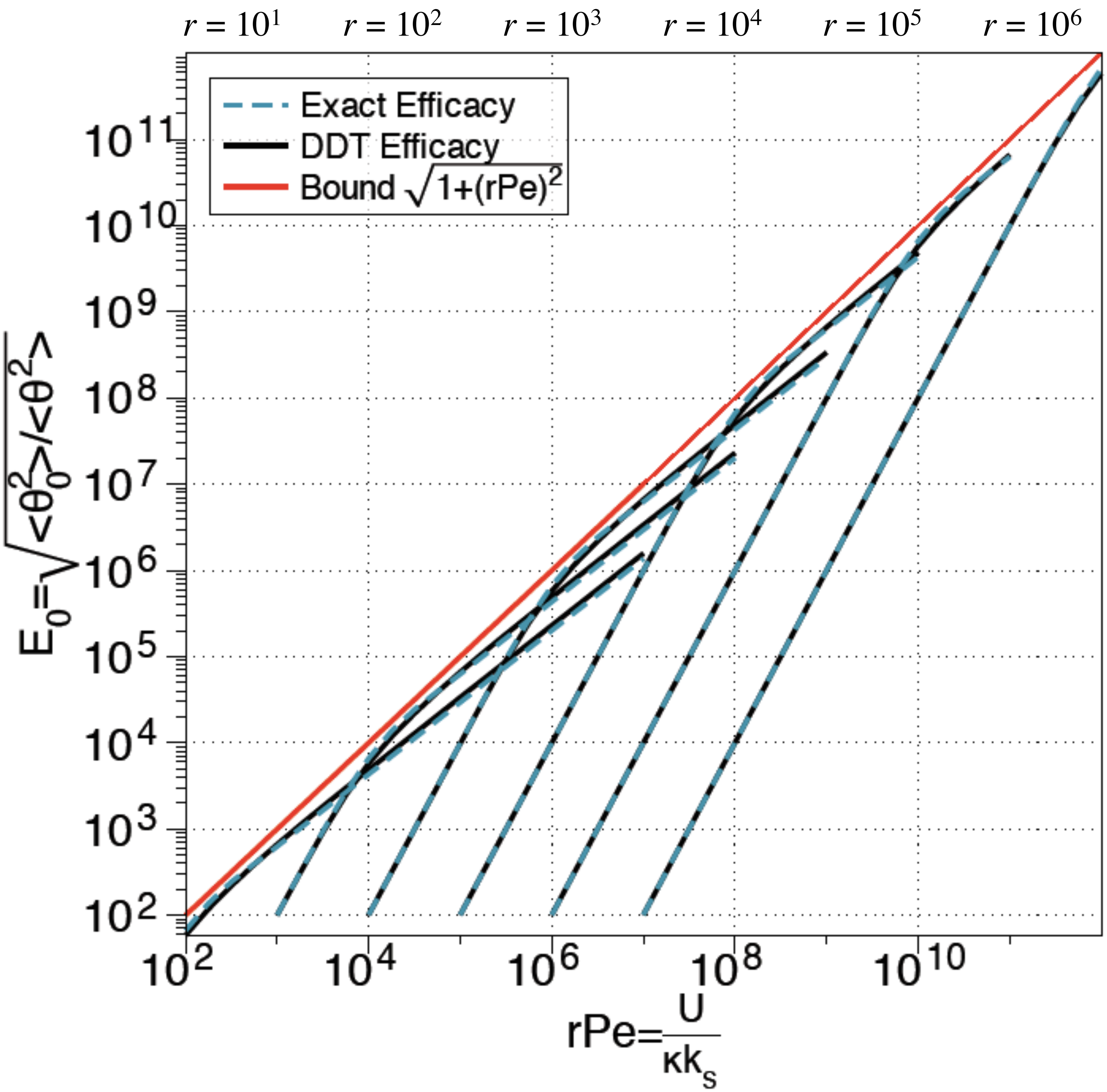
- DDT respects the rigorous bounds on κ_0^{VR}.

- For the single-scale source, the rigorous bound is

$$E(\mathrm{Pe}) = \kappa_0^{\mathrm{VR}} / \kappa \leq [1 + r^2 \mathrm{Pe}^2]^{1/2} \sim r\,\mathrm{Pe} \ldots$$

… for large r or for large Pe!

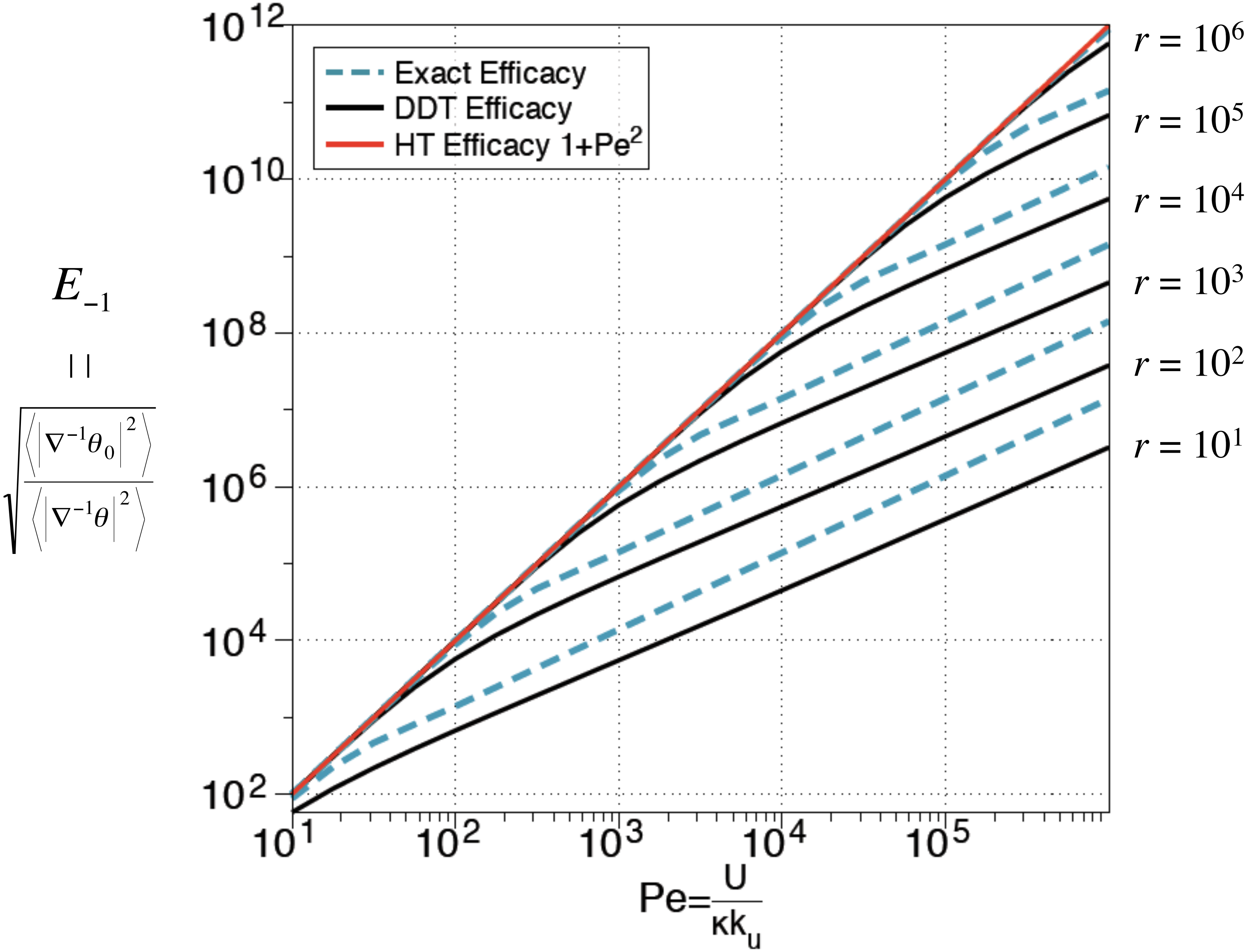
- Plot E(Pe) as a function of (rPe):



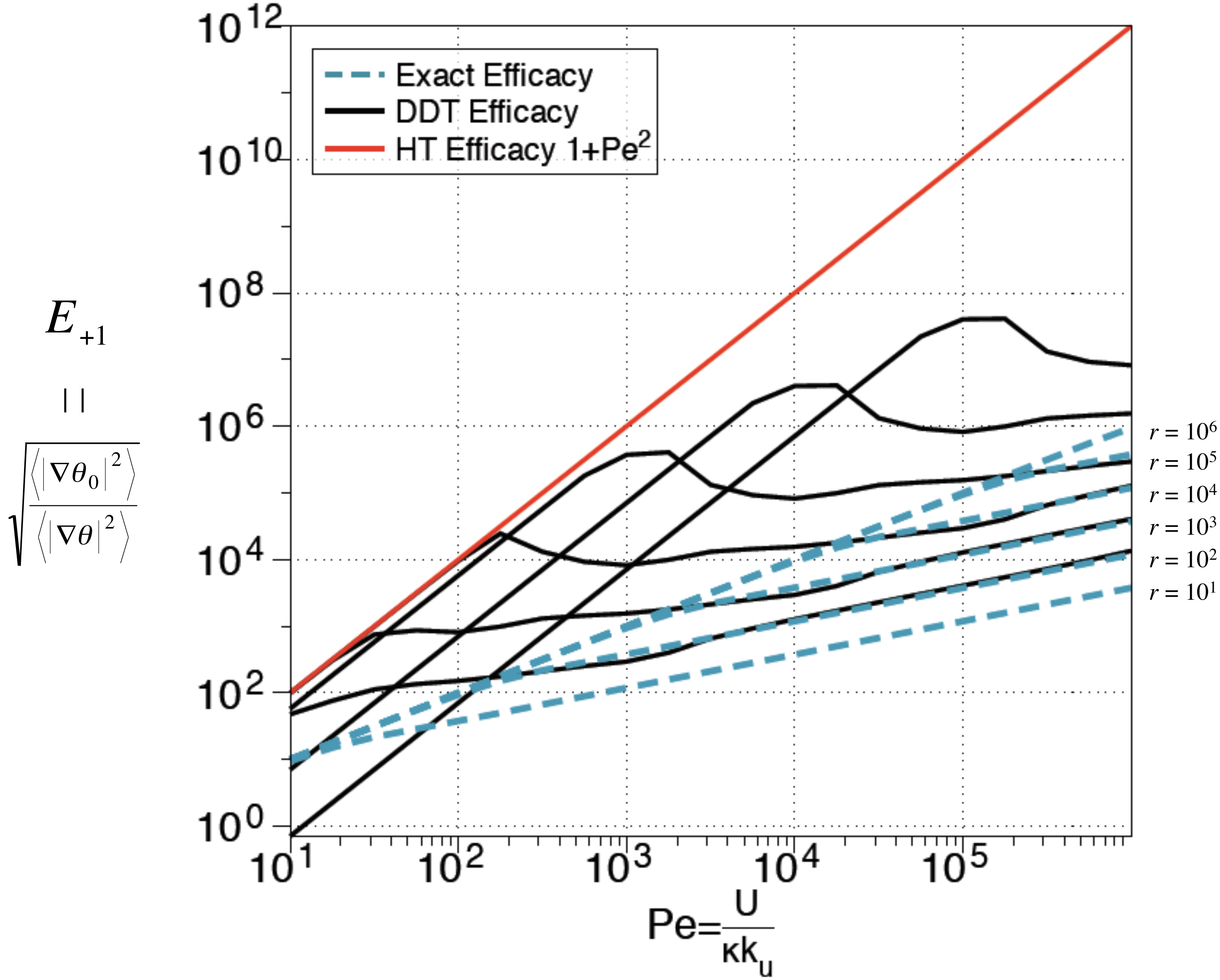
r = 10^1
r = 10^2
r = 10^3
r = 10^4
r = 10^5
r = 10^6
Exact Efficacy
DDT Efficacy
Bound √(1+(rPe)^2)
E_0=√(<θ_0^2>/<θ^2>)
rPe=U/(κk_s)
10^2
10^3
10^4
10^5
10^6
10^7
10^8
10^9
10^10
10^11
10^2
10^4
10^6
10^8
10^10

Reconciliation, continued

- How does DDT perform for variance supression at large & small scales, i.e., for $\kappa_{\pm 1}{}^{VR}$?

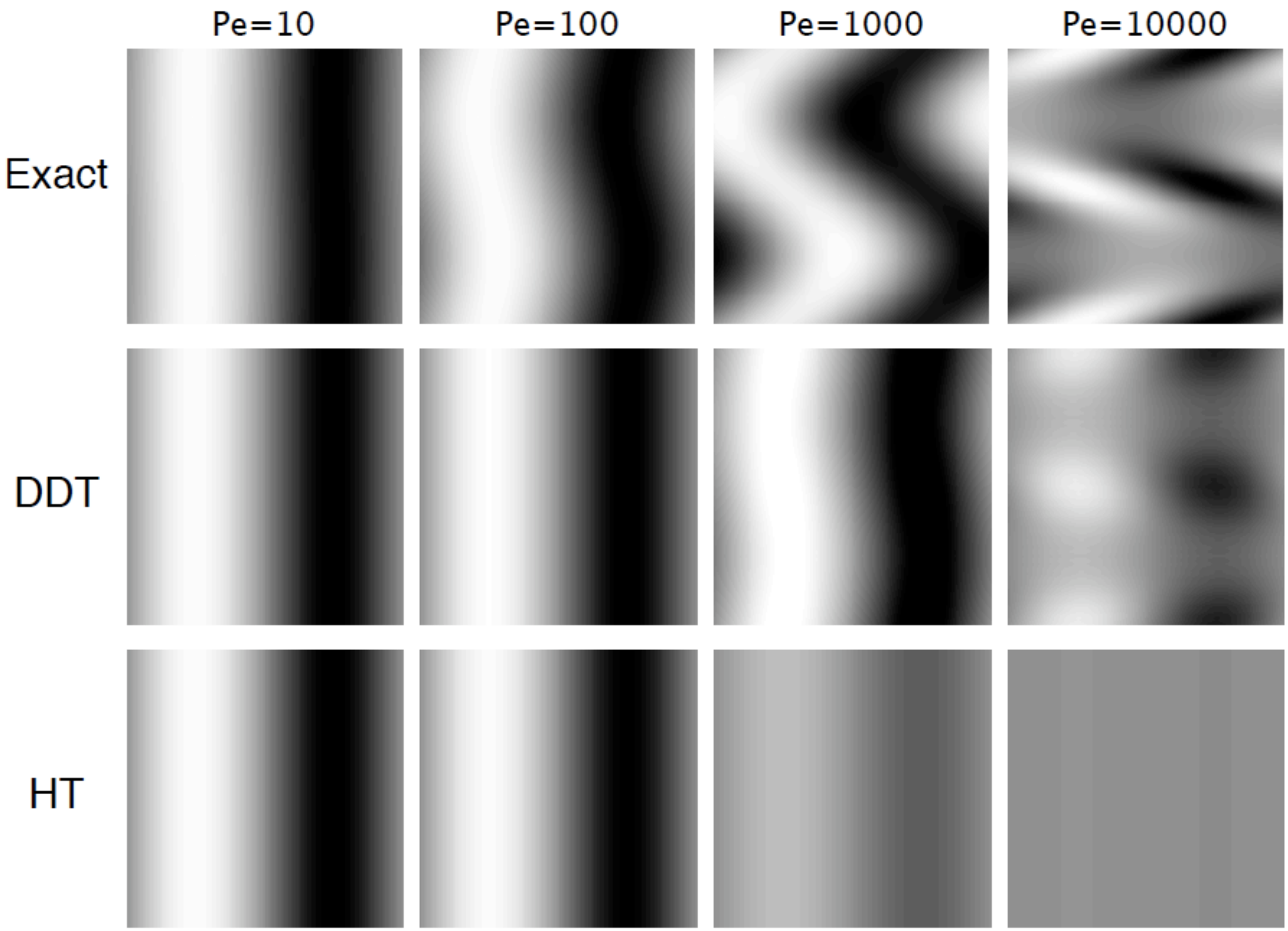


Exact Efficacy
DDT Efficacy
HT Efficacy 1+Pe^2
$r = 10^6$
$r = 10^5$
$r = 10^4$
$r = 10^3$
$r = 10^2$
$r = 10^1$
$E_{-1} = \sqrt{\frac{\langle |\nabla^{-1}\theta_0|^2 \rangle}{\langle |\nabla^{-1}\theta|^2 \rangle}}$
$\mathrm{Pe} = \frac{U}{\kappa k_u}$
10^2 10^4 10^6 10^8 10^{10} 10^{12}
10^1 10^2 10^3 10^4 10^5

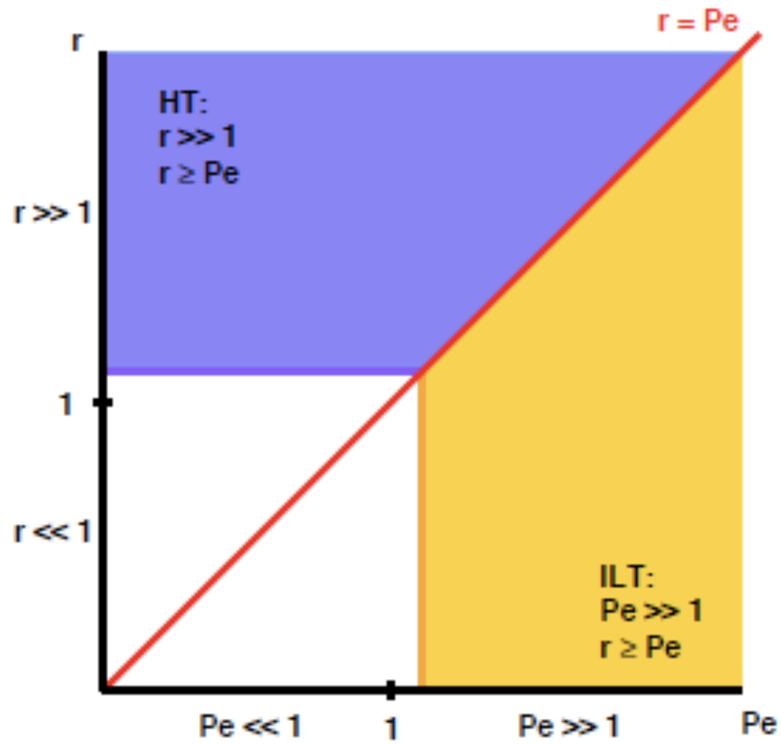


Exact Efficacy
DDT Efficacy
HT Efficacy 1+Pe^2
$E_{+1} = \sqrt{\frac{\langle|\nabla\theta_0|^2\rangle}{\langle|\nabla\theta|^2\rangle}}$
$\mathrm{Pe}=\frac{U}{\kappa k_u}$
$r = 10^6$
$r = 10^5$
$r = 10^4$
$r = 10^3$
$r = 10^2$
$r = 10^1$
10^{0}
10^{2}
10^{4}
10^{6}
10^{8}
10^{10}
10^{12}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}

Density pictures ($r = 562$)



Stirring strength–scale separation phase diagram



DDT approximation for κ_0^{VR} is uniformly accurate

Conjecture (potential application)

- Single-scale source, sink & stirring is a special scenario …

  … what about ***real*** turbulent mixing?

- DDT hints how particle dispersion data may predict steady state source-sink sustained variance suppression.

- Homogeneous isotropic turbulence →

$$\mathrm{E}[(\mathrm{X}_i(t)\text{–}\mathrm{X}_i(0))(\mathrm{X}_j(t)\text{–}\mathrm{X}_j(0))] = (2\kappa t + U^2t^2 + C_R\,\varepsilon t^3 + \ldots)\,\delta_{ij}$$

… w/turbulent energy dissipation rate per unit mass $\varepsilon \sim U^3/\ell_{flow}$.

On a periodic domain $[0,L]^d$

$$\rho(\vec{x},t \mid \vec{x}_0,t_0) \approx \frac{1}{L^d}\sum_{\vec{k}} \exp\left\{i\vec{k}\cdot(\vec{x}-\vec{x}_0) - \tfrac{1}{2}k^2\left[2\kappa(t-t_0) + U^2(t-t_0)^2 + \cdots\right]\right\}$$

$$\theta_{\text{DDT}}(\vec{x},t) = \int_{-\infty}^{t} dt_0 \int d\vec{x}_0\, \rho(\vec{x},t \mid \vec{x}_0,t_0)\, s(\vec{x}_0)$$

$$\Downarrow$$

$$\hat{\theta}_{\text{DDT}}(\vec{k}) = \hat{s}(\vec{k}) \int_0^{\infty} e^{-\kappa k^2 \tau - \frac{1}{2}k^2 U^2 \tau^2}\, d\tau$$

$$\Rightarrow \text{ as } \mathrm{Pe} = \frac{U\ell_{flow}}{\kappa} \to \infty \text{ at fixed } r = \frac{\ell_{source}}{\ell_{flow}},$$

$$\hat{\theta}_{\text{DDT}}(\vec{k}) \sim \frac{\hat{s}(\vec{k})}{k\,U}$$

Concrete conjecture:

Does Statistically Homogeneous

Isotropic Turbulence saturate

the upper bound on $E(\mathrm{Pe})$?

$$\kappa^{eff} \text{ approximated by } \kappa_0^{VR} = \sqrt{\frac{\left\langle \left(\Delta^{-1} s\right)^2 \right\rangle}{\left\langle \theta_{\mathrm{DDT}}^2 \right\rangle}} \sim \kappa \, r \, \mathrm{Pe} \quad \hookleftarrow$$

$$= \left(\frac{\ell_{source}}{\ell_{flow}} \right) U \ell_{flow}$$

$$\text{with } \ell_{source} = \left(\frac{\left\langle \left(\Delta^{-1} s\right)^2 \right\rangle}{\left\langle \left(\Delta^{-1/2} s\right)^2 \right\rangle} \right)^{1/2}$$

i.e., "mixing length" $\sim \ell_{source}$

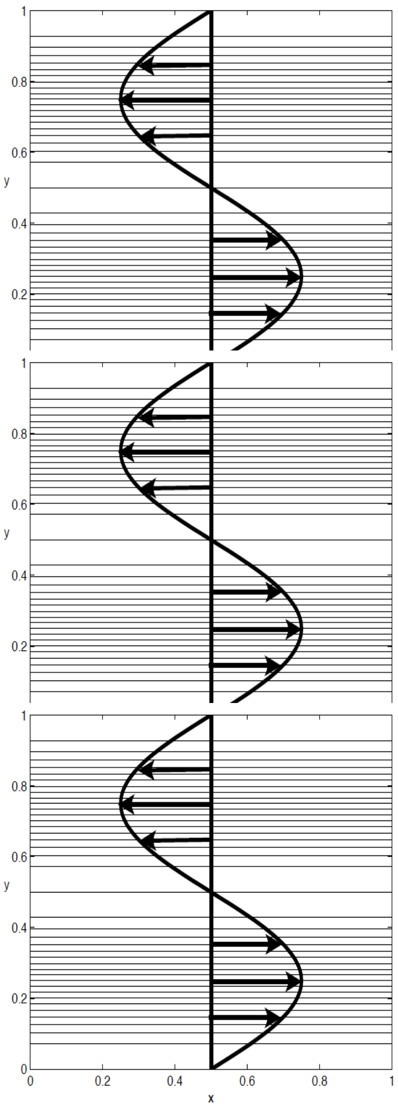
$$\Rightarrow \text{ as } \mathrm{Pe}=\frac{U\ell_{flow}}{\kappa} \rightarrow \infty \text{ at fixed } r=\frac{\ell_{source}}{\ell_{flow}},$$

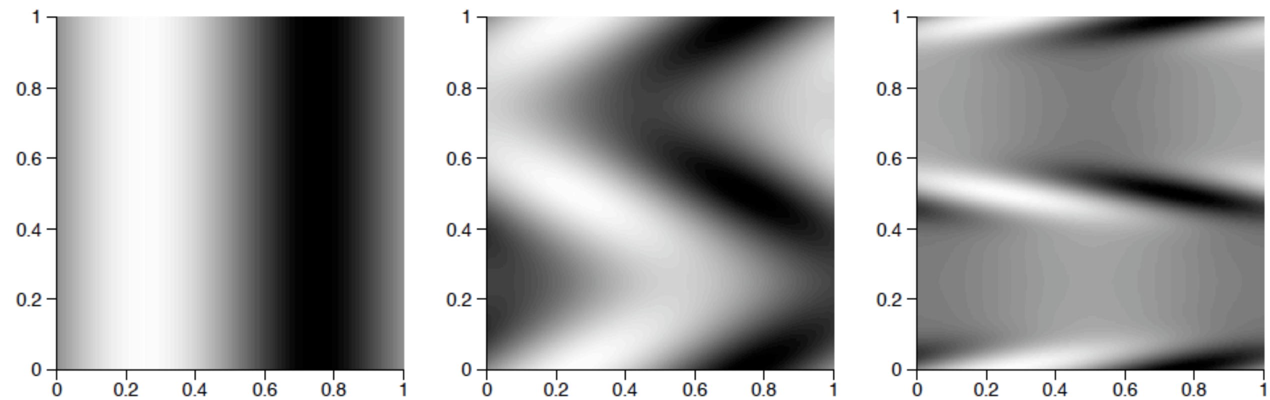
$$\hat{\theta}_{\mathrm{DDT}}(\vec{k}) \sim \frac{\hat{s}(\vec{k})}{k\,U}$$

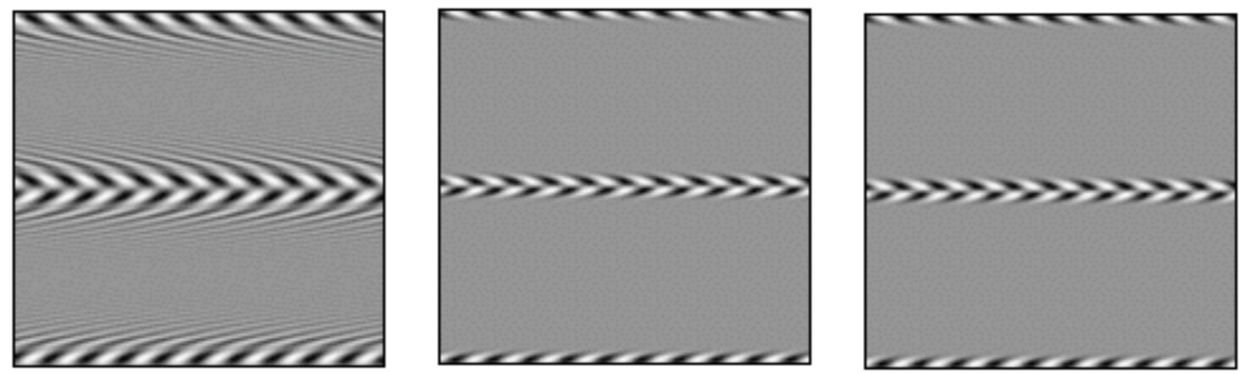
Last words

- Different definitions of effective diffusion may indeed yield different effective diffusivities.
- We cannot generally use long-time transient dispersion results for source-sink problems.
- There may not be an effective diffusion equation to describe source-sink stirring.
- Flux-gradient model does not contain all the relevant information for source-sink stirring.
- Transient mixing and source-sink stirring are ***different phenomena*** using ***different features*** of the flow:

Scalar source-sink stirring is all about ***transport***







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Dynamics of probability density functions for decaying passive scalars in periodic velocity fields

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Transient mixing is all about

shearing, stretching & straining

THE END