# Accurate numerical integral method for computing drift-kinetic Rosenbluth potentials*

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# NIMROD implements a drift kinetic field operator*

$$
\begin{aligned}
C_{ab}^{\text{field}} &= \Gamma_{ab}\left\{4\pi\frac{m_a}{m_b}f_b + \left(\frac{m_a}{m_b}-1\right)\frac{2v}{v_{Ta}^2}\frac{\partial H_b}{\partial v} + \frac{2v^2}{v_{Ta}^4}\frac{\partial^2 G_b}{\partial v^2} - \frac{2}{v_{Ta}^2}H_b\right\}f_a^{\text{M}} \\
G_b\left(v,\xi\right) &= 4v^4\int_0^\infty d\bar{v}\bar{v}^{5/2}\int_{-1}^{1}d\xi' F_b\left(v\bar{v},\xi'\right)E\left(k\right)\sqrt{\bar{v}^{-1}+\bar{v}-2\xi\xi'+2\sqrt{1-\xi^2}\sqrt{1-\xi'^2}} \\
H_b\left(v,\xi\right) &= 4v^2\int_0^\infty d\bar{v}\bar{v}^{3/2}\int_{-1}^{1}d\xi' F_b\left(v\bar{v},\xi'\right)K\left(k\right)/\sqrt{\bar{v}^{-1}+\bar{v}-2\xi\xi'+2\sqrt{1-\xi^2}\sqrt{1-\xi'^2}}
\end{aligned}
$$

where

$$\bar{v} = v'/v$$

$$k = \sqrt{4\sqrt{1-\xi^2}\sqrt{1-\xi'^2}/\left(\bar{v}^{-1}+\bar{v}-2\xi\xi'+2\sqrt{1-\xi^2}\sqrt{1-\xi'^2}\right)}$$

Gauss-Chebyshev for $\int d\bar{v}$ and native Gauss-Legendre or GLL for $\int d\xi'$

*E. D. Held, *et al*, Phys Plasmas **22**, 032511 (2015).

# Finite element method discretizes pitch-angle

$$F_a(\xi, s, t) = \sum_l F_{a,l}(s,t)\, P_l(\xi)$$ where $P_l(\xi)$ are GLL elements or Legendre polynomials

Integrals used in field operator

$$E_{ll'}(\bar{v}) = \int_{-1}^{1} d\xi \int_{-1}^{1} d\xi' P_l(\xi)\, P_{l'}(\xi')\, 4\bar{v}^{5/2} E(k)\, \frac{\sqrt{4\sqrt{1-\xi^2}\sqrt{1-\xi'^2}}}{k}$$

$$K_{ll'}(\bar{v}) = \int_{-1}^{1} d\xi \int_{-1}^{1} d\xi' \frac{P_l(\xi)\, P_{l'}(\xi')\, 4\bar{v}^{3/2} k K(k)}{\sqrt{4\sqrt{1-\xi^2}\sqrt{1-\xi'^2}}}$$

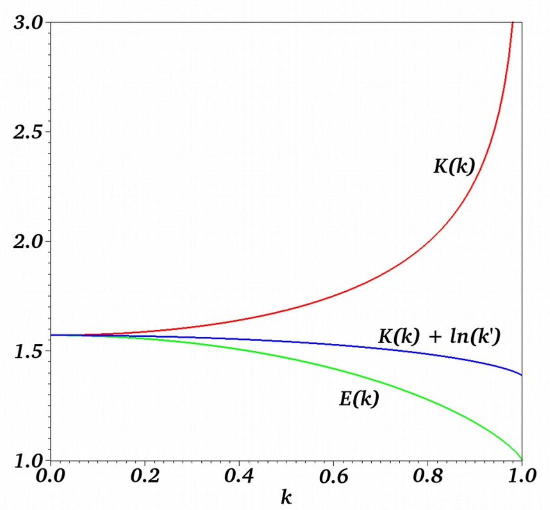
$$K'_{ll'}(\bar{v}, \xi, \xi') = \int_{-1}^{1} d\xi \int_{-1}^{1} d\xi' \frac{2\left(\bar{v}^{5/2} - \bar{v}^{1/2}\right) P_l(\xi)\, P_{l'}(\xi')\, E(k) / \left(1-k^2\right)}{\left(\bar{v} + \bar{v}^{-1} - 2\xi\xi' + 2\sqrt{(1-\xi'^2)(1-\xi^2)}\right)^{3/2}}$$

$$E''_{ll'}(\bar{v}) = \frac{1}{2}\bar{v}\left[\left(\bar{v}^{-1} + \bar{v}\right) K_{ll'}(\bar{v}) - \left(\bar{v} - \bar{v}^{-1}\right) K'_{ll'}(\bar{v})\right]$$

# $\xi/\xi'$ integrals regularized by splitting technique*

$$\int d\xi' \frac{P_{l'}\left(\xi'\right) kK\left(k\right)}{\sqrt{4\sqrt{1-\xi^2}\sqrt{1-\xi'^2}}} =$$

$$\overbrace{\int d\xi' \left[ \frac{P_{l'}\left(\xi'\right) kK\left(k\right)}{\sqrt{4\sqrt{1-\xi^2}\sqrt{1-\xi'^2}}} + \frac{P_{l'}\left(\xi\right) \ln\left(\frac{\sqrt{1-k^2}}{4}\right)}{\sqrt{\bar{v}+\bar{v}^{-1}+2-4\xi^2}} \right]}^{\text{Numerical}} - \frac{P_{l'}\left(\xi\right) \overbrace{\int d\xi' \ln\left(\frac{\sqrt{1-k^2}}{4}\right)}^{\text{Analytical}}}{\sqrt{\bar{v}+\bar{v}^{-1}+2-4\xi^2}}$$




$$\int d\xi' \frac{P_{l'}\left(\xi'\right) E\left(k\right) / \left(1-k^2\right)}{\left(\bar{v}+\bar{v}^{-1}-2\xi\xi'+2\sqrt{1-\xi^2}\sqrt{1-\xi'^2}\right)^{3/2}} =$$

$$\overbrace{\int d\xi' \left\{ \frac{P_{l'}\left(\xi'\right) E\left(k\right) / \left(1-k^2\right)}{\left(\bar{v}+\bar{v}^{-1}-2\xi\xi'+2\sqrt{1-\xi^2}\sqrt{1-\xi'^2}\right)^{3/2}} + \frac{2\bar{v}P_{l'}\left(\xi\right)}{\bar{v}^{-1}-\bar{v}} \frac{\partial}{\partial \bar{v}} \left[ \frac{\ln\left(\frac{\sqrt{1-k^2}}{4}\right)}{\sqrt{\bar{v}+\bar{v}^{-1}+2-4\xi^2}} \right] \right\}}^{\text{Numerical}} - \frac{2\bar{v}P_{l'}\left(\xi\right)}{\bar{v}^{-1}-\bar{v}} \frac{\partial}{\partial \bar{v}} \overbrace{\left[ \frac{\int d\xi' \ln\left(\frac{\sqrt{1-k^2}}{4}\right)}{\sqrt{\bar{v}+\bar{v}^{-1}+2-4\xi^2}} \right]}^{\text{Analytical}}$$

*Inspired by J. M. Huré, Astronomy & Astrophysics, 434, 1 (2005).

# Analytic integral used for regularization

$$
\int_{\xi_a}^{\xi_b} d\xi' \ln\left(\frac{\sqrt{1-k^2}}{4}\right) =
$$

$$
\Re e\left\{\frac{\xi\sqrt{1-\xi^2}+ic\sqrt{c^2-1}}{c^2-\xi^2}\zeta\times\right.
$$

$$
\left[\ln\left(\frac{\left(\xi_b-c\xi+i\sqrt{(1-\xi^2)(c^2-1)}\right)\zeta\sqrt{1-\xi_b^2}+i\sqrt{(1-\xi^2)(c^2-1)}\left(1-\xi_b^2\right)+(c-\xi\xi_b)(c\xi_b-\xi)}{(c-\xi\xi_b)^2-(1-\xi^2)(1-\xi_b^2)}\right)\right.
$$

$$
\left.\left.-\ln\left(\frac{\left(\xi_a-c\xi+i\sqrt{(1-\xi^2)(c^2-1)}\right)\zeta\sqrt{1-\xi_a^2}+i\sqrt{(1-\xi^2)(c^2-1)}\left(1-\xi_a^2\right)+(c-\xi\xi_a)(c\xi_a-\xi)}{(c-\xi\xi_a)^2-(1-\xi^2)(1-\xi_a^2)}\right)\right]\right\}
$$

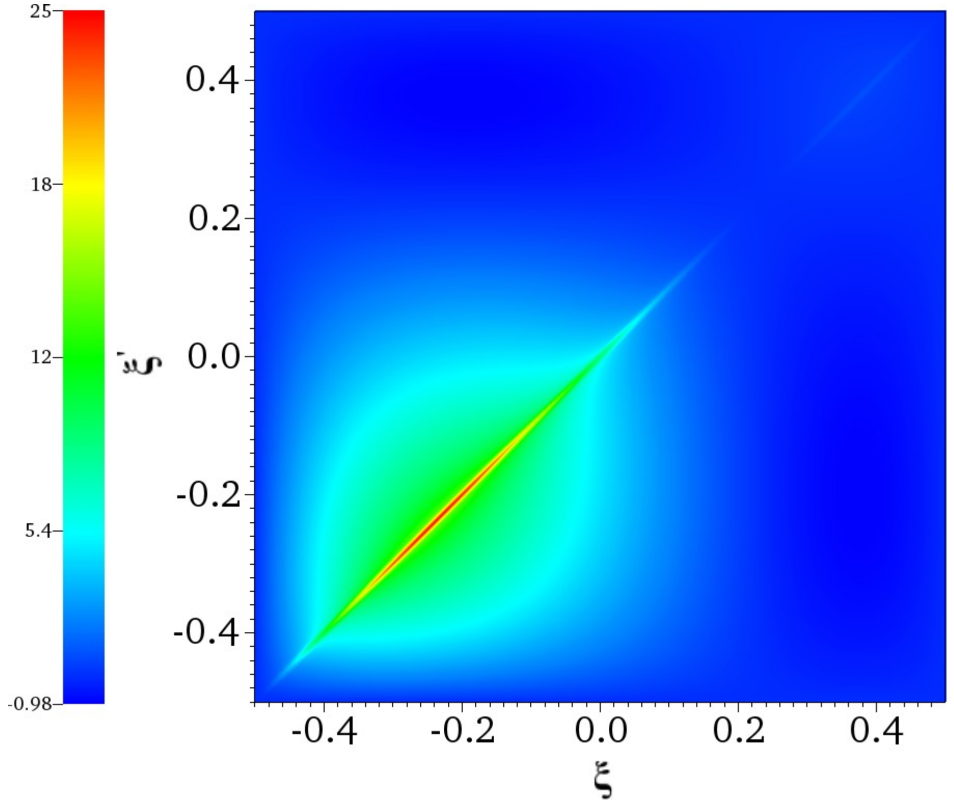
$$
+\frac{\xi_b}{2}\ln\left(\frac{c-\xi\xi_b-\sqrt{(1-\xi^2)(1-\xi_b^2)}}{c-\xi\xi_b+\sqrt{(1-\xi^2)(1-\xi_b^2)}}\right)-\frac{\xi_a}{2}\ln\left(\frac{c-\xi\xi_a-\sqrt{(1-\xi^2)(1-\xi_a^2)}}{c-\xi\xi_a+\sqrt{(1-\xi^2)(1-\xi_a^2)}}\right)
$$

$$
-\ln(4)(\xi_b-\xi_a)-c\sqrt{1-\xi^2}\left(\sin^{-1}\xi_b-\sin^{-1}\xi_a\right)
$$

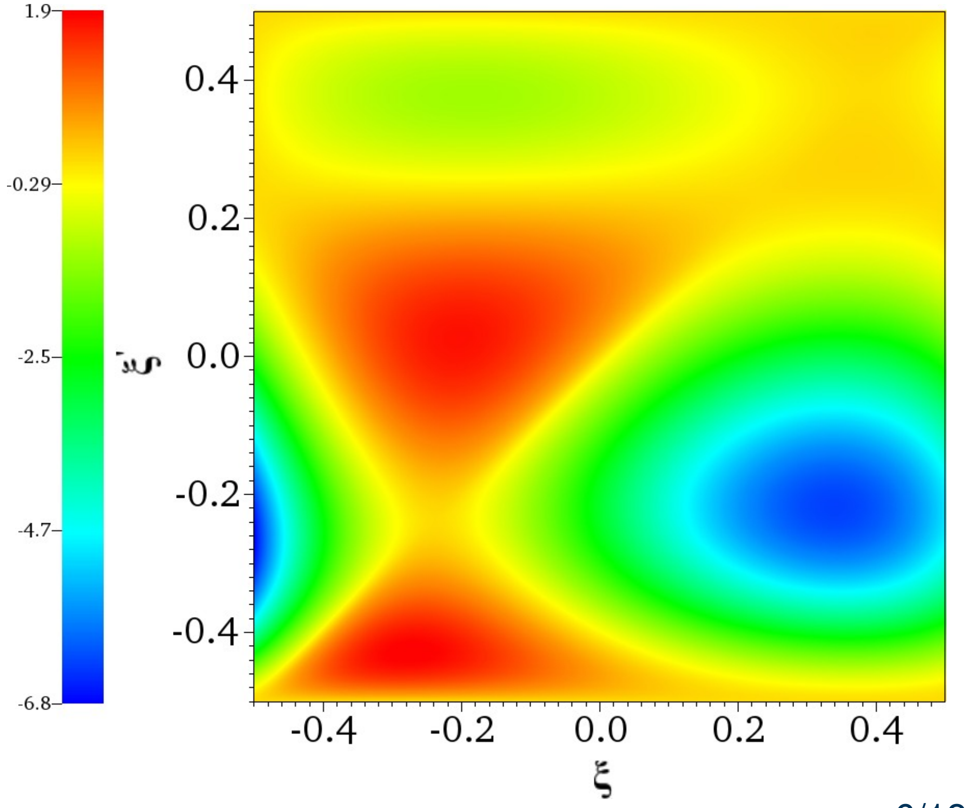
where $\quad c=\dfrac{\bar{v}^{-1}+\bar{v}}{2}, \qquad \zeta\equiv\sqrt{1-\left(c\xi+i\sqrt{(1-\xi^2)(c^2-1)}\right)^2}.$

# Example of regularized integrand using numerical splitting technique

Original $K_{5,5}\,(\bar{v} = 0.99995)$ integrand

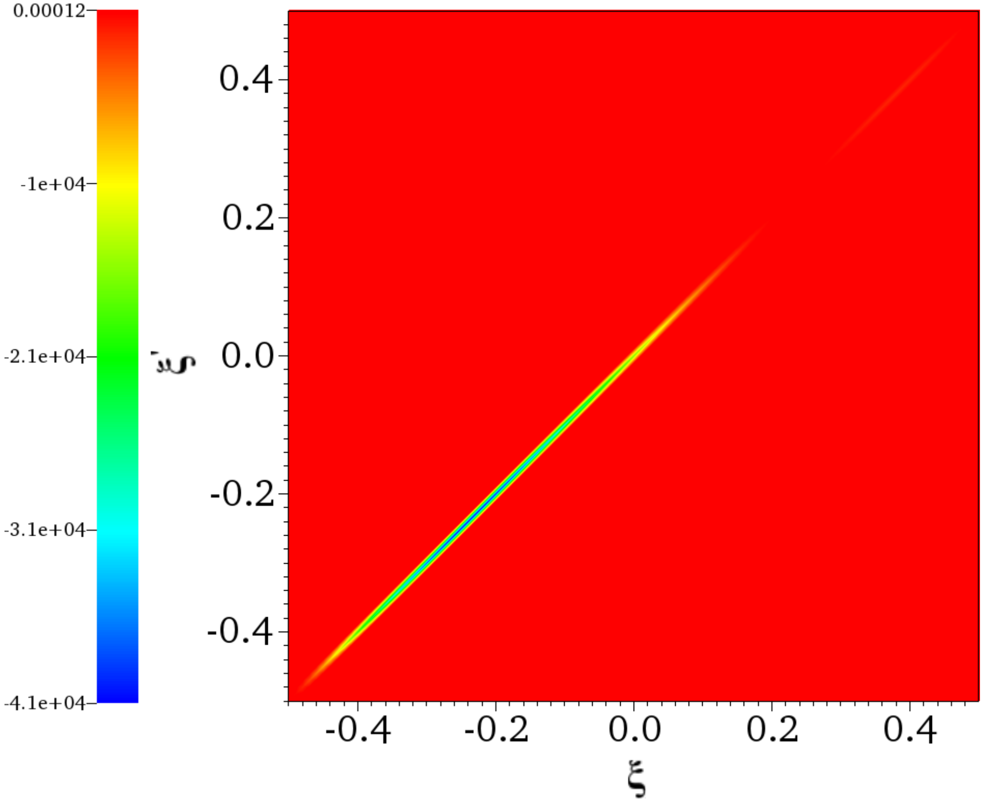



Residual $K_{5,5}\,(\bar{v} = 0.99995)$ integrand

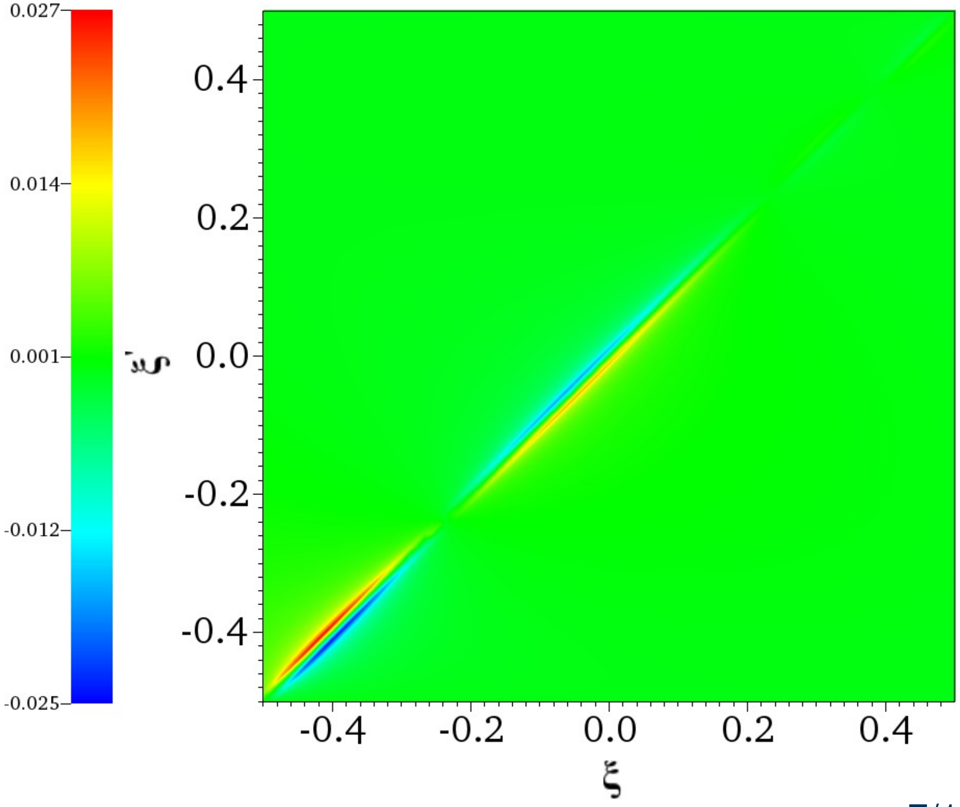


# Example of regularized integrand using numerical splitting technique

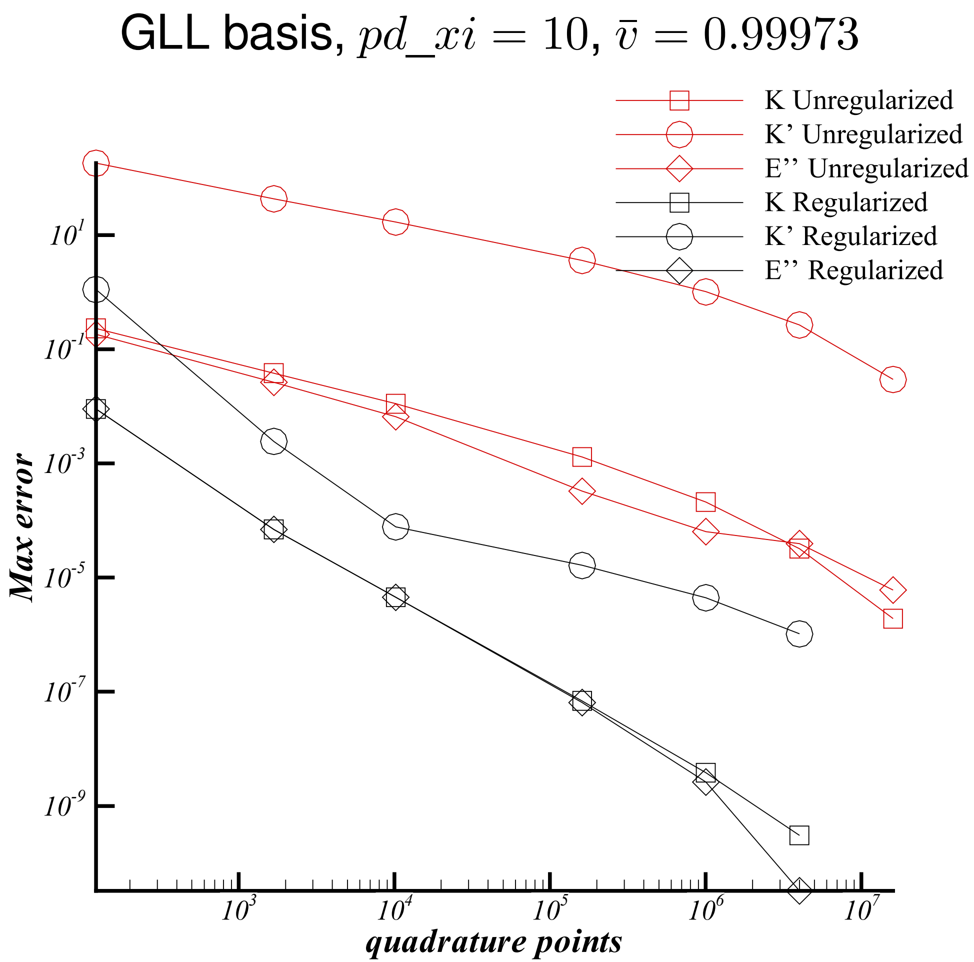
Original $K'_{5,5}$ $(\bar{v} = 0.99995)$ integrand

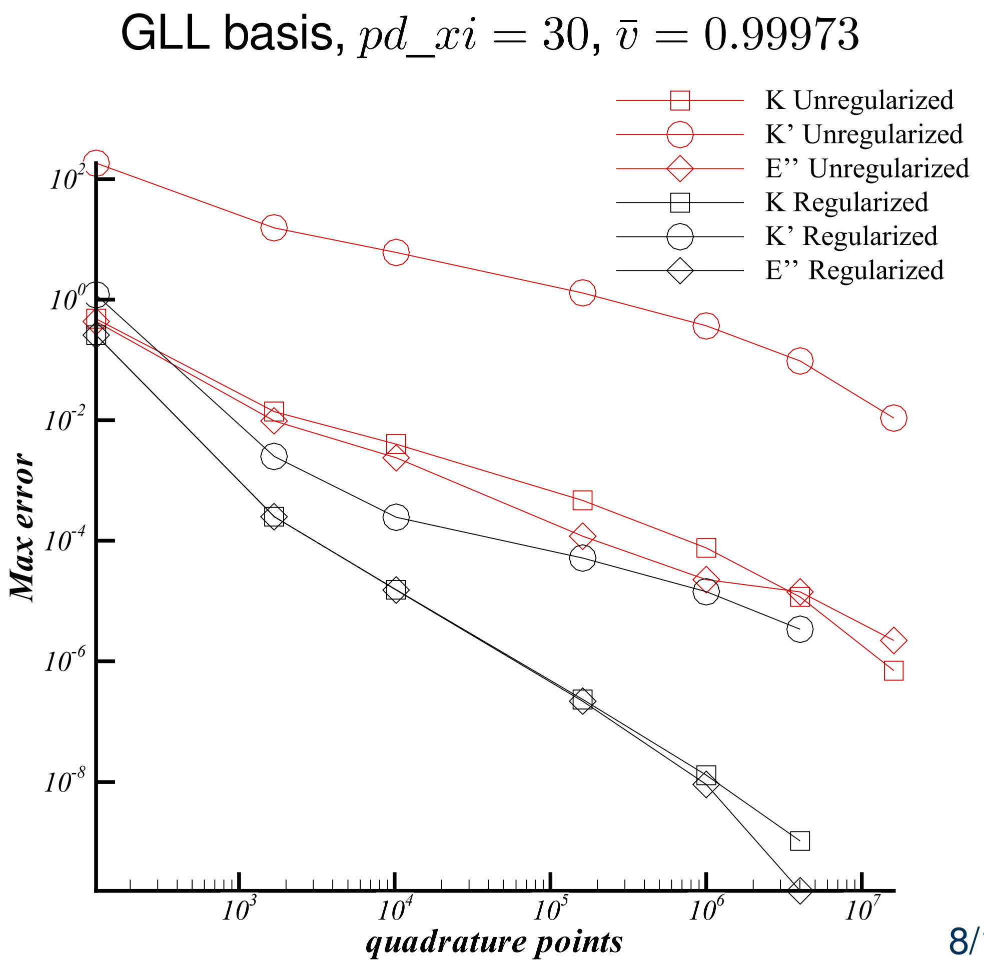



Residual $K'_{5,5}$ $(\bar{v} = 0.99995)$ integrand



# Regularization improves accuracy



# Collocation method discretizes speed

Let $s \equiv v/v_{Ta}$, $f_0(s) = e^{-s^2}$, and $\chi = v_{Tb}/v_{Ta}$

$$F_a(s) = \sum_{k=0}^{N_s-1} F^*_{a,k} f_0(s) L_k(s), \qquad F^*_{a,k} = \sum_j w_j L_k(s_j) F_a(s_j)$$

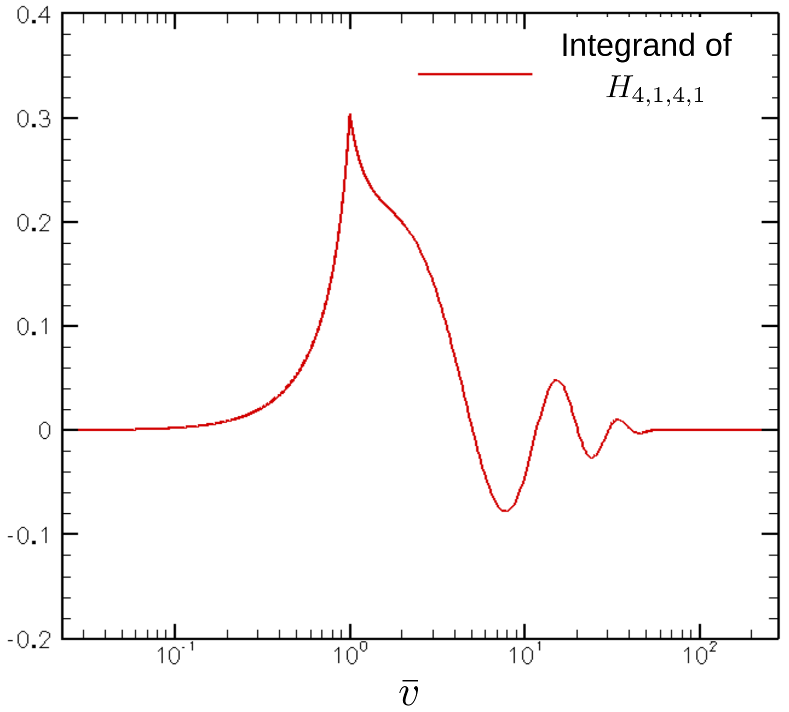
Integrate over $\bar{v} \in (0,1)$, $\bar{v} \in (1,2)$, and $\bar{v} \in (2,\infty)$ seperately.

$$H_{b,l,i,l',j} = v_{Ta}^2 s_i^2 \int_0^\infty d\bar{v} \sum_{k=0}^{N_s-1} w_j L_k(s_j) f_0\left(\bar{v}\frac{s_i}{\chi}\right) L_k\left(\bar{v}\frac{s_i}{\chi}\right) K_{ll'}(\bar{v})$$

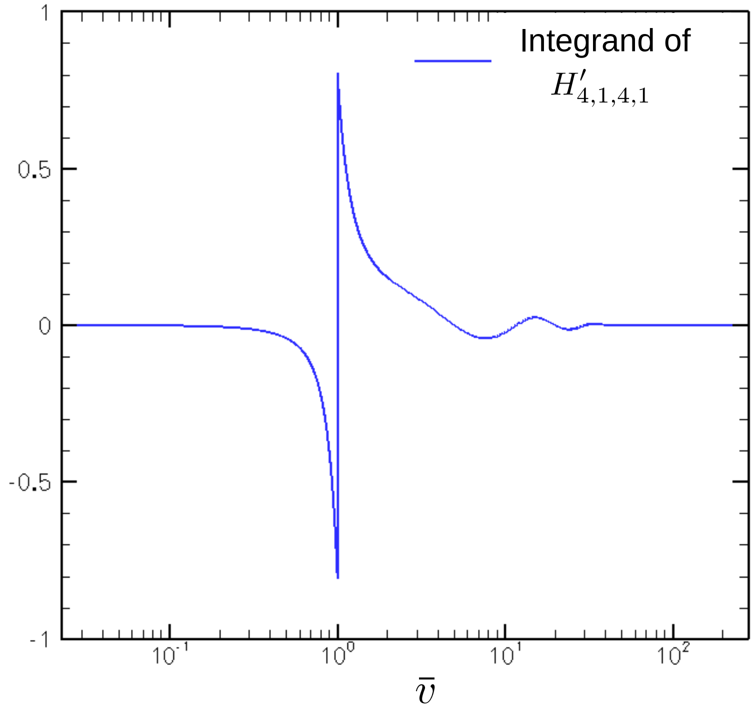
$$H'_{b,l,i,l',j} = v_{Ta} s_i \int_0^\infty d\bar{v} \sum_{k=0}^{N_s-1} w_j L_k(s_j) f_0\left(\bar{v}\frac{s_i}{\chi}\right) L_k\left(\bar{v}\frac{s_i}{\chi}\right) K'_{ll'}(\bar{v}) - \frac{H_{b,l,i,l',j}}{2v_{Ta}s_i}$$

$$G''_{b,l,i,l',j} = v_{Ta}^2 s_i^2 \int_0^\infty d\bar{v} \sum_{k=0}^{N_s-1} w_j L_k(s_j) f_0\left(\bar{v}\frac{s_i}{\chi}\right) L_k\left(\bar{v}\frac{s_i}{\chi}\right) E''_{ll'}(\bar{v}) - \frac{G_{b,l,i,l',j}}{4v_{Ta}^2 s_i^2}$$

# Singular behavior at v=v'

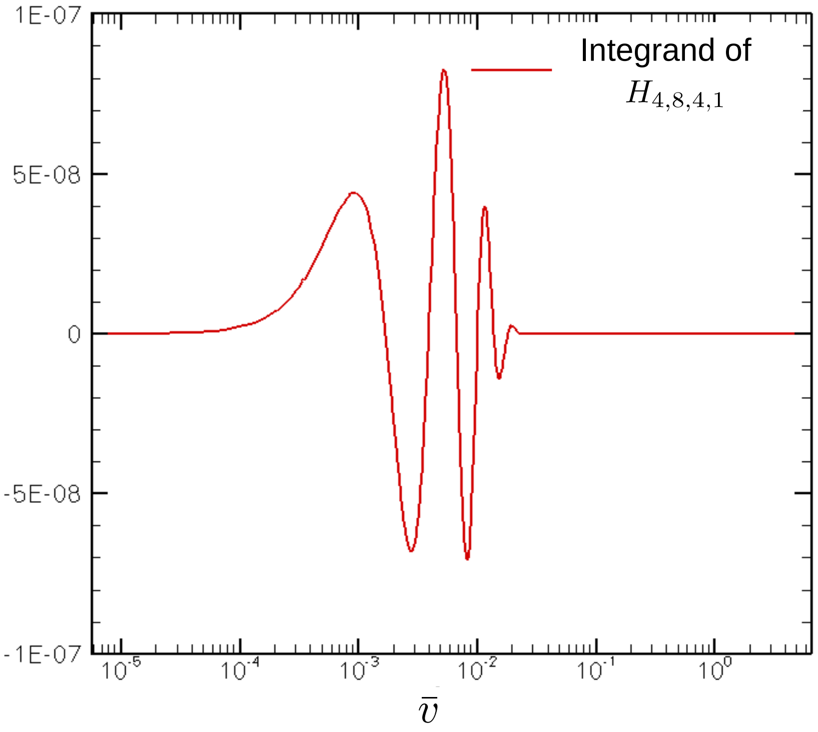



Integrand of $H$ with $l = 4,\ l' = 4,\ i = 1,\ j = 1$ for like-species collisions.

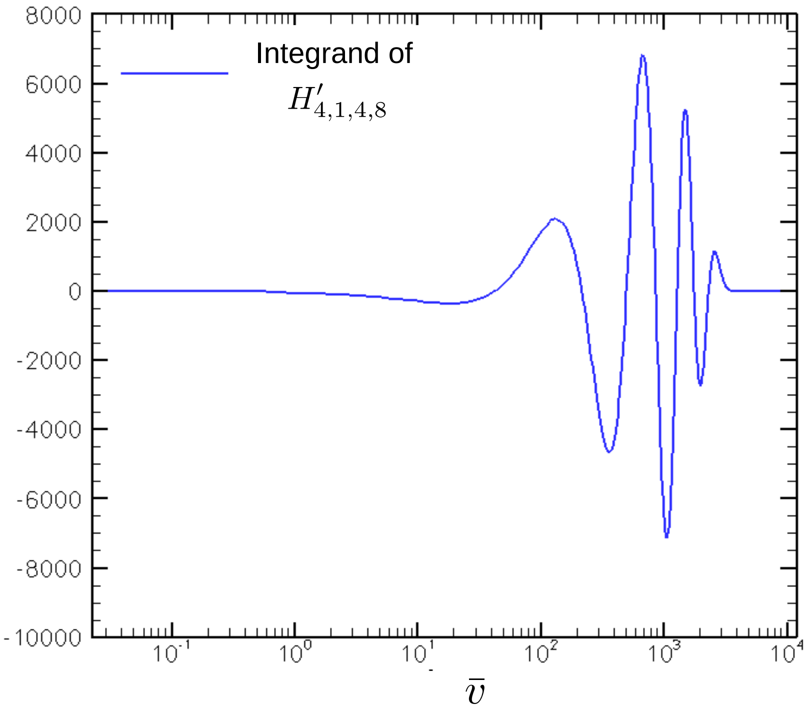



Integrand of $H'$ with $l = 4,\ l' = 4,\ i = 1,\ j = 1$ for like-species collisions.

# Response at low and high vbar




Integrand of $H$ with $l = 4,\ l' = 4,\ i = 8,\ j = 1$ for electron-ion collisions.




Integrand of $H'$ with $l = 4,\ l' = 4,\ i = 1,\ j = 8$ for ion-electron collisions.

# Addressing vbar=1

For $\bar{v} \in (1,2)$ and $\bar{v} \in (1,2)$, we need packing near $\bar{v} = 1$:

1) Gauss-Chebyshev quadrature

$$f_0 \equiv \frac{1}{\sqrt{1-\bar{v}^2}}$$

Map nodes and weights from $-1 \to 1$ and $0 \to 2$.

2) Nonclassical Gaussian quadrature with weight function

$$f_0 \equiv \frac{1}{|1-\bar{v}|}$$

3) Nonclassical Gaussian quadrature with weight function

$$f_0 \equiv \frac{e^{-\left(\bar{v}\frac{s_i}{\chi}\right)^2}}{|1-\bar{v}|}$$

# Addressing high vbar

1) Use Gauss-Legendre quadrature for $\bar{v} \in (2, \bar{v}_{\text{max}})$.

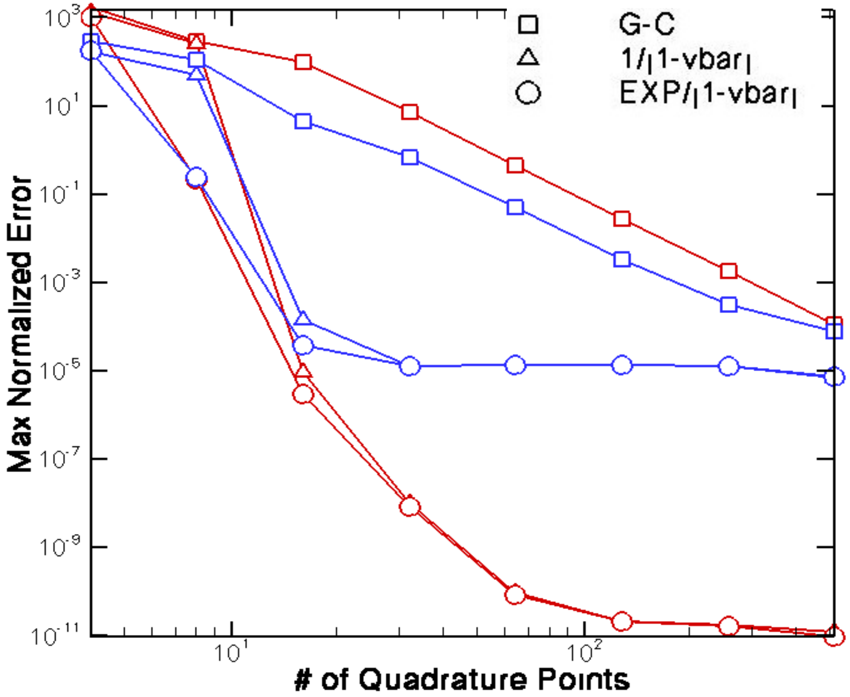
2) Nonclassical Gaussian quadrature with weight function

$$f_0 \equiv e^{-\left(\bar{v}\frac{s_i}{\chi}\right)^2}$$

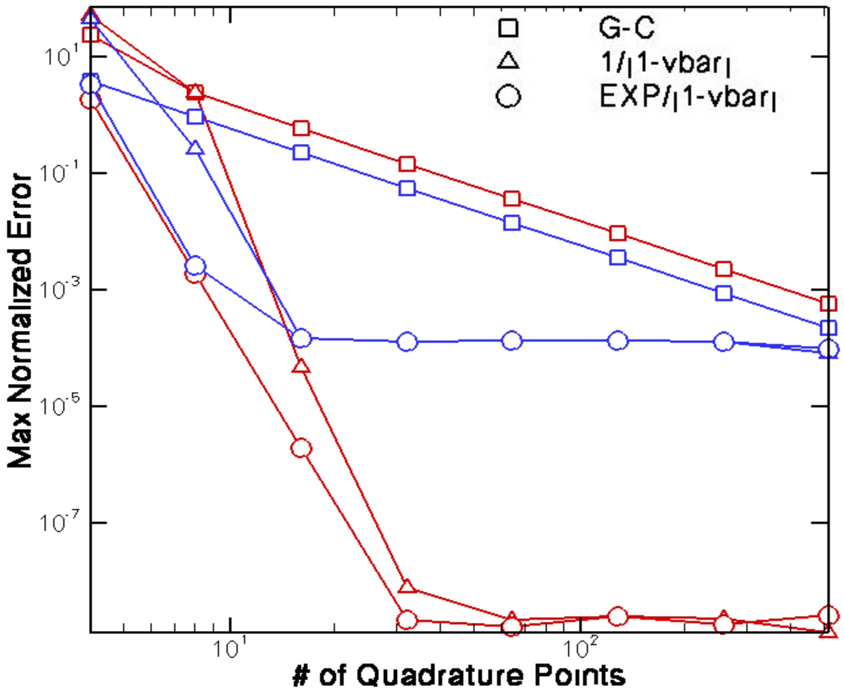
3) Since this requires a separate quadrature scheme for each outer speed point, try to get around this by using the $i = 1$ weight for all of them.

$$f_0 \equiv e^{-\left(\bar{v}\frac{s_1}{\chi}\right)^2}$$

# Convergence behavior

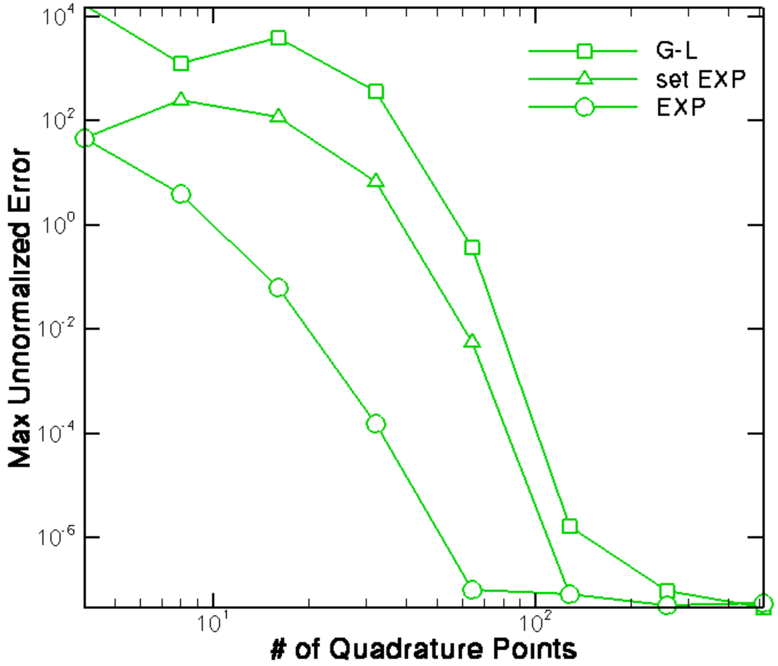



Maximum error of contribution to $H_{l,i,l',j}$ (red) and $H'_{l,i,l',j}$ (blue) from the integral over $\bar{v} \in (0,1)$ for like-species collisions.

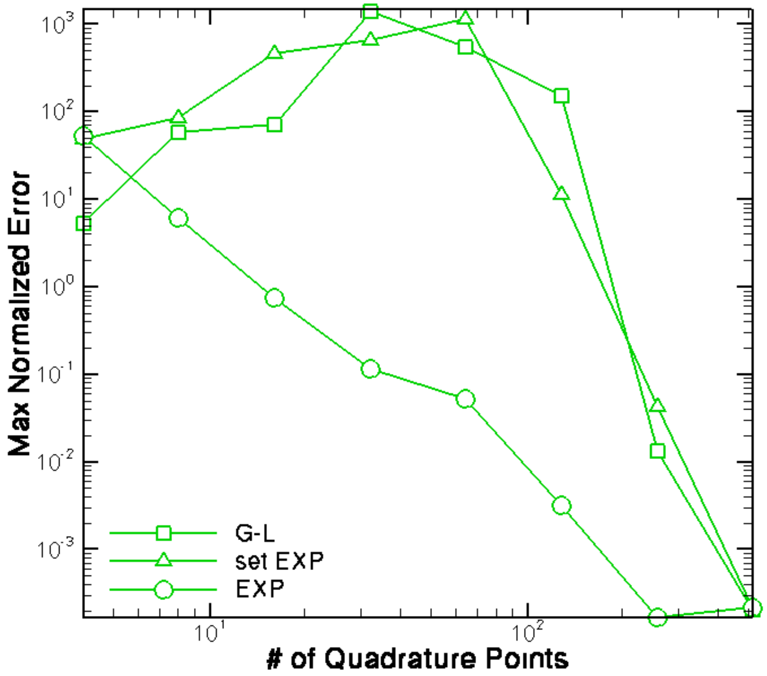



Maximum error of contribution to $H_{l,i,l',j}$ (red) and $H'_{l,i,l',j}$ (blue) from the integral over $\bar{v} \in (1,2)$ for like-species collisions.

# Convergence behavior

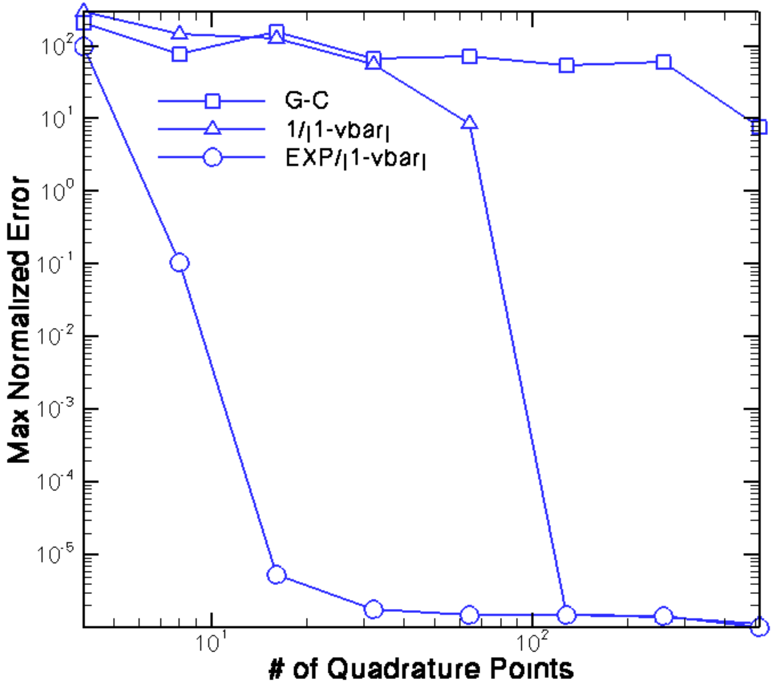



Maximum error of contribution to $G''_{l,i,l',j}$ from the integral over $\bar{v} \in (2, \infty)$ for like-species collisions.

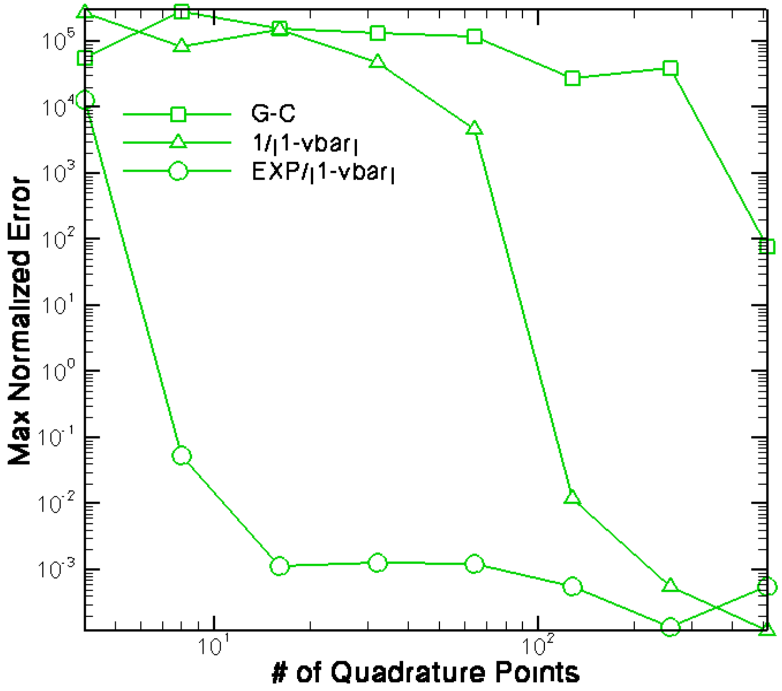



Maximum error of contribution to $G''_{l,i,l',j}$ from the integral over $\bar{v} \in (2, \infty)$ for ion-electron collisions.

# Convergence behavior




Maximum error of contribution to $H'_{l,i,l',j}$ from the integral over $\bar{v} \in (0,1)$ for electron-ion collisions.




Maximum error of contribution to $G''_{l,i,l',j}$ from the integral over $\bar{v} \in (0,1)$ for electron-ion collisions.

# Conclusions

- For $\bar{v} \in (2, \infty)$, nonclassical Gaussian quadrature with $f_0 = \exp(-(\bar{v}s_i/\chi)^2$ is most accurate.
  - Too expensive, so use $f_0 = \exp\left(-(\bar{v}s_1/\chi)^2\right)$ instead.

- For $\bar{v} \in (0, 1)$ and $\bar{v} \in (2, \infty)$, nonclassical Gaussian quadrature with $f_0 = 1/|1-\bar{v}|$ is best.

- Can accurately compute the moments.
- Still very costly.

# Future work

- Explore ways to further improve $\xi,\xi'$ integration scheme:
  - Regularize integrals at $\xi,\xi' = \pm 1$
  - Regularize off-diagonal cells near $\xi = \xi'$
- Try different $\xi,\xi'$ quadrature scheme
  - Romberg integration, or use adaptive integration software
- Explore ways to analytically compute the couplings for $\bar{v} >> 1$ and $\bar{v} << 1.$
  - Expand the integrand in series using the parameter $c \equiv \bar{v} + \dfrac{1}{\bar{v}}.$
- Implement preassigned node for continuity at boundary of the two speed domains.
- Test on the Spitzer thermalization and conduction problems.