Collisionality dependence of impurity transport in Alcator C-Mod H-modes

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Recent experiments have been performed to collect a data set over wide range of collisionality, explore collisionality dependence of H-mode impurity transport

Outline

- Electron density peaking in H-mode
- Initial look at global confinement trends
- Measuring impurity transport coefficients on C-Mod
- New analysis/uncertainty quantification techniques
- Initial look at core transport coefficient profiles
H-mode electron density peaking scales with collisionality

Cross-machine scaling law [1, 2]

\[ \frac{n_e(0)}{\langle n_e \rangle} \text{ scales with } \nu_{\text{eff}} = 0.1Z_{\text{eff}}R \frac{\langle n_{e,19} \rangle}{\langle T_{e,\text{keV}} \rangle^2} \]

This scaling enables interesting studies of impurity transport

- Explore connection between electron and impurity peaking.
- Actuate the neoclassical pinch and turbulence drive (both \( \propto \nabla n_e \)), explore implications for high-\( Z \) accumulation [3].

[3] Reinke et al., JI1.00002 (tuesday PM)
Initial look at global confinement

- All discharges are EDA H-modes: no ELMs, pedestal regulated by quasi-coherent mode (QCM).
- Scanned $I_p$ to vary $\langle n_e \rangle$, scanned $P_{ICRF}$ to vary $\langle T_e \rangle$.
- Strong scaling with $(\nabla n_e)_{\text{ped}}$ consistent with J. Rice, PO3.00004 (earlier this session).
- Challenge: extract local core transport information from plasma with global confinement dominated by pedestal.
Alcator C-Mod is uniquely equipped to make detailed measurements of impurity transport

- Multipulse laser blow-off impurity injector can inject Ca (or other desired impurity) multiple times per shot [1].
- X-ray imaging crystal spectrometer [2] observes spatial profile of a single charge state (Ca$^{18+}$): more direct interpretation than unresolved soft x-rays.
- Result is strongly sensitive to background $n_e$, $T_e$ profiles.

[1] Howard et al. (2011), RSI
[2] Ince-Cushman et al. (2008), RSI
[3] Howard et al. (2012), NF
New techniques for uncertainty propagation

- Profile fitting is fundamental to transport analysis.
- Splines are bad at finding uncertainty in gradient.
- New approach [1]: Gaussian process regression (GPR) [2]
  - Automatic, delivers reliable uncertainty estimate for gradient.
  - Based on spatial covariance of data points, not an assumed functional form.
  - Output is probability distribution (PDF), can be efficiently propagated through subsequent analysis.

$y$: observation, $y_*$: prediction

$$f(y_*, y = 1) = \frac{f(y_*, y = 1)}{f(y = 1)}$$

conditional posterior

"PDF of $y_*$ given $y"$

Joint prior

marginal prior

$$f(y) = \int f(y_*, y) dy_*$$

contours: joint prior PDF

solid: marginal prior PDF

dashed: conditional posterior PDF

solid: marginal prior PDF

contours: joint prior PDF

Solid: marginal prior PDF

Dashed: conditional posterior PDF

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2. Rasmussen and Williams, Gaussian Processes for Machine Learning, MIT Press, 2006
Example: Fitting an H-mode density profile

Open source software available: github.com/markchil/gptools/
Preliminary analysis yields H-mode core impurity transport coefficient profiles

- Reconstruction not reliable for $r/a > 0.6$.
- High $D$ inside inversion radius could simply be result of incomplete handling of sawteeth, further analysis is necessary.
- Core impurity transport dominated by anomalous diffusivity.
Alcator C-Mod’s combination of powerful diagnostics, novel analysis techniques and reactor-relevant conditions enables detailed study of H-mode impurity transport

Summary

- Scaling of electron density peaking with $\nu_{\text{eff}}$ provides convenient actuator for $a/L_{ne}$: vary neoclassical pinch and turbulence drive.
- Have made detailed measurements of impurity transport in EDA H-modes of varying $\nu_{\text{eff}}$.
- Reconstruction of $D$, $V$ profiles has begun.
- New data analysis techniques have been developed to fit profiles, efficiently propagate uncertainty.

Future Work

- Analyze more shots with different collisionalities.
- Compare to gyrokinetic simulations.
Backup slides

1. Gaussian processes

2. gp tools

3. Bayesian inference
The hyperparameters can be estimated by maximizing the likelihood

Likelihood of the training data given \( k \) with hyperparameters \( \theta = [\sigma_f, \ell, \ldots] \):

\[
\ln p(y|X, \theta) = -\frac{1}{2} y^T [K + \Sigma_n]^{-1} y - \frac{1}{2} \ln |K + \Sigma_n| - \frac{n}{2} \ln 2\pi
\]

- Maximize with respect to hyperparameter vector \( \theta \).
- Local maxima: different possible interpretations of the data. E.g., noisy and long-\( \ell \) versus precise and short-\( \ell \)
- Compare likelihoods to select the most appropriate kernel.
Full treatment of hyperparameters uses MCMC integration
Point estimate misses substantial uncertainty in gradient

<table>
<thead>
<tr>
<th>Quantity</th>
<th>$y$</th>
<th>$y'$</th>
<th>$a/L_y$</th>
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</thead>
<tbody>
<tr>
<td>$n_e$, MAP</td>
<td>1.2%</td>
<td>6.0%</td>
<td>6.0%</td>
</tr>
<tr>
<td>$n_e$, MCMC</td>
<td>1.4%</td>
<td>8.4%</td>
<td>8.3%</td>
</tr>
<tr>
<td>$T_e$, MAP</td>
<td>1.3%</td>
<td>3.7%</td>
<td>4.0%</td>
</tr>
<tr>
<td>$T_e$, MCMC</td>
<td>1.4%</td>
<td>5.4%</td>
<td>5.6%</td>
</tr>
</tbody>
</table>
Bad versus good choices for the hyperparameters have a large effect on the likelihood

\[
\begin{align*}
\text{Initial} & \quad \ln p = -29.1 \\
\text{Optimal} & \quad \ln p = -3.0
\end{align*}
\]
Getting gradients and their uncertainties is straightforward.

The derivative of a GP is a GP:

\[
\text{cov} \left( y_i, \frac{\partial y_j}{\partial x_{dj}} \right) = \frac{\partial k(x_i, x_j)}{\partial x_{dj}}
\]

\[
\text{cov} \left( \frac{\partial y_i}{\partial x_{di}}, \frac{\partial y_j}{\partial x_{dj}} \right) = \frac{\partial^2 k(x_i, x_j)}{\partial x_{di} \partial x_{dj}}
\]

- Derivative equality constraint: just add a datapoint!
- Derivative predictions: predictive distribution contains the uncertainty.
Capturing the pedestal requires a non-stationary kernel

Gibbs kernel: \( \ell \) is an arbitrary function of \( x \)

\[
k_G(x, x') = \sigma_f^2 \left( \frac{2 \ell(x) \ell(x')}{\ell^2(x) + \ell^2(x')} \right)^{1/2} \exp \left( -\frac{|x - x'|^2}{\ell^2(x) + \ell^2(x')} \right)
\]

Complete \( n_e \) profile: Gibbs covariance kernel

- **Length scale:**
  \[
  \ell = \frac{\ell_1 + \ell_2}{2} - \frac{\ell_1 - \ell_2}{2} \tanh \frac{x - x_0}{\ell_w}
  \]

- **Handled** \( \ell_1, \ell_2, \ell_w \) and \( x_0 \) by maximizing \( \ln p \) (MAP) and by marginalizing with MCMC.
Gibbs kernel with tanh length scale has been extensively tested with noisy synthetic data.
Error estimates from Gibbs kernel with tanh length scale have been shown to be asymptotically consistent using noisy synthetic data.

Asymptotic consistency of GPR fits

(a) value

(b) gradient

RMS error vs. number of points
gptools: An extensible, object-oriented Python package for multivariate GPR including gradients

- Available GPR codes lack one or more critical features:
  - Ability to both constrain and predict gradients.
  - Straightforward way to draw random samples.
- gptools was written to meet these needs:
  - Object-oriented structure.
  - Interface for easy data fusion and application of constraints.
  - SE, Gibbs, Matérn and RQ kernels with support for arbitrary orders of differentiation.
- Available on GitHub: www.github.com/markchil/gptools
gptools contains two classes for performing GPR

<table>
<thead>
<tr>
<th>GaussianProcess</th>
<th>Kernel</th>
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<tbody>
<tr>
<td>k : Kernel</td>
<td>num_dim</td>
</tr>
<tr>
<td>nk : Kernel</td>
<td>params</td>
</tr>
<tr>
<td>X</td>
<td>fixed_params</td>
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<td>n</td>
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<tr>
<td>y</td>
<td></td>
</tr>
<tr>
<td>err_y</td>
<td></td>
</tr>
<tr>
<td>add_data(X, y, err_y, n)</td>
<td><strong>call</strong>(Xi, Xj, ni, nj)</td>
</tr>
<tr>
<td>optimize_hyperparameters()</td>
<td>set_hyperparams(new_params)</td>
</tr>
<tr>
<td>predict(X_star)</td>
<td></td>
</tr>
<tr>
<td>draw_sample(X_star)</td>
<td></td>
</tr>
</tbody>
</table>
import gptools

# Create kernel:
k = gptools.SquaredExponentialKernel(1)

# Create GP:
gp = gptools.GaussianProcess(k, X=R_mid, y=Te, err_y=err_Te)

# Impose zero slope constraint at magnetic axis:
gp.add_data(R_mag, 0, n=1)

# Optimize hyperparameters:
gp.optimize_hyperparameters()

# Make a prediction of the value:
R_star = scipy.linspace(R_mag, R_mid.max(), 100)
Te_fit, Te_std = gp.predict(R_star)

# Make a prediction of the gradient:
gradTe_fit, gradTe_std = gp.predict(R_star, n=1)
gptools implements a very general form of GPR

\[ f \left( \begin{bmatrix} M_* \\ M \end{bmatrix} \right) = \mathcal{N} \left( \begin{bmatrix} T_* & 0 \\ 0 & T \end{bmatrix} \begin{bmatrix} \mu(X_*) \\ \mu(X) \end{bmatrix}, \begin{bmatrix} T_* & 0 \\ 0 & T \end{bmatrix} \begin{bmatrix} K(X_*, X_*) & K(X_*, X) \\ K(X_*, X) & K(X, X) \end{bmatrix} \begin{bmatrix} T_*^T & 0 \\ 0 & T^T \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ 0 & \Sigma_M \end{bmatrix} \right) \]

\[
\ln L = -\frac{n}{2} \ln 2\pi - \frac{1}{2} \ln \left| TK(X, X)T^T + \Sigma_M \right|
- \frac{1}{2} (M - T\mu(X))^T (TK(X, X)T^T + \Sigma_M)^{-1} (M - T\mu(X))
\]

\[
f(M_* | M) = \mathcal{N}(T_*\mu(X_*), T_*K(X_*, X)T^T (TK(X, X)T^T + \Sigma_M)^{-1} (M - T\mu(X)))
- T_*K(X_*, X_*)T_*^T - T_*K(X_*, X)T^T (TK(X, X)T^T + \Sigma_M)^{-1} TK(X, X_*)T_*^T)
\]

- Supports data of arbitrary dimension \( x \in \mathbb{R}^n \).
- Supports explicit, parametric mean function \( \mu(x) \): can perform nonlinear regression with GP fit to residuals.
- Supports arbitrary linear transformations \( T, T_* \) of inputs, outputs: can perform tomographic inversions constrained with point measurements.
- Supports noise of arbitrary structure \( \Sigma_M \) on observations.
GPR: a probabilistic method to fit profiles

\[
f(y_*|y = 1) = \frac{f(y_*, y = 1)}{f(y = 1)}
\]

conditional posterior
"PDF of \( y_* \) given \( y \)"

- Create multivariate normal prior distribution that sets smoothness, symmetry, etc.
- **Condition** on observations to yield the fit, including uncertainty estimate.
- Distribution can include derivatives, line integrals, volume averages, etc.
The properties of the fit are inferred using Bayes’ rule

Given spatial covariance characterized by hyperparameter vector \( \theta \) and observations \( y \), Bayes’ rule is:

\[
f(\theta|y) = \frac{\text{likelihood} \cdot \text{prior}}{\text{evidence}} = \frac{f(y|\theta)}{f(y)} f(\theta)
\]

- **Likelihood**: Probability of observing the data \( y \) given the hyperparameters \( \theta \). Simply a multivariate normal for GPR.
- **Prior**: Distribution encoding any prior assumptions about the hyperparameters \( \theta \) (positivity, typical values, etc.)
- **Evidence**: Probability of the data under the model. Just a normalization constant for parameter estimation.
- **Posterior**: Probability distribution for the hyperparameters \( \theta \) given the data \( y \): the end-goal of the inference.
Three levels of sophistication to select hyperparameters $\theta$

$$f(\theta | y) = \frac{\text{likelihood} \cdot \text{prior}}{f(y)}$$

**so-so:** **Maximum likelihood** (ML): Pick the hyperparameters $\theta$ that maximize the likelihood $f(y | \theta)$ of the data.

**better:** **Maximum a posteriori** (MAP, “empirical Bayes”): Pick the hyperparameters $\theta$ that have the highest posterior probability $f(\theta | y)$.

**best:** **Marginalization** (“full Bayes”): Average over the possible hyperparameters when making a prediction $y^*$:

$$f(y^* | y) = \int f(y^* | y, \theta) f(\theta | y) \, d\theta$$